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(54) Title: CRYSTAL STRUCTURE OF BACE AND USES THEREOF

(57) Abstract: This invention is directed to the three dimensional crystal structure of Beta-site APP Cleaving Enzyme (BACE), and to the use of this structure in rational drug design methods to identify agents that may interact with active sites of BACE. Such agents may represent new therapeutics in the treatment and/or prevention of Alzheimer's Disease.

CRYSTAL STRUCTURE OF BACE AND USES THEREOF

Field of the Invention

[0001] The present invention relates to the three dimensional crystal structure of Beta-site APP Cleaving Enzyme (BACE), and to the use of this structure in rational drug design methods to identify agents that may interact with active sites of BACE. Such agents may represent new therapeutics in the treatment and/or prevention of Alzheimer's Disease.

Background of the Invention

[0002]A characteristic pathology of Alzheimer's Disease is the build up of insoluble amyloid plaques in the brain. These proteinaceous plaques are composed of a 4KDa, 42 amino acid fragment of β-Amyloid Precursor Protein (APP) and is termed Amyloid β -peptide (A β). The mechanism of A β production is hence of critical importance in understanding the onset and progress of Alzheimer's Disease. It has been shown that $A\beta$ is derived from the proteolytic cleavage of a larger protein, β -amyloid precursor protein (APP). Two enzymes are responsible for this cleavage; first, the enzyme β -secretase cleaves APP at residue 671 (770aa isoform of APP numbering) and then γ-secretase cleaves at residue 716. More recently, the novel transmembrane aspartic protease BACE has been identified as being β -secretase. This protein is now a significant target in a therapeutic approach to Alzheimer's Disease. In rare cases of Alzheimer's Disease that are hereditary (Familial Alzheimer's Disease (FAD)) the disease phenotype has been isolated to mutations in the β -Amyloid Precursor Protein. One particular cohort, the 'Swedish mutation', exhibits a double mutation at the β -secretase cleavage site.

[0003] Based upon the role of BACE in Alzheimer's Disease, the elucidation of the three-dimensional structure of BACE, as well as its site of binding with APP, would have important implications in the treatment and/or prevention of Alzheimer's Disease and similar diseases associated with the

presence of insoluble amyloid plaques composed the 42 amino acid fragment of APP in the brain.

Summary of the Invention

In the present invention provides a crystal of BACE complexed with an APP inhibitor peptide, as well as the three dimensional structure of BACE as derived by x-ray diffraction data of the BACE/APP inhibitor peptide crystal. Specifically, the three dimensional structure of BACE is defined by the structural coordinates shown in Figure 1, ± a root mean square deviation from the backbone atoms of the amino acids of not more than 1.5Å. The structural coordinates of BACE are useful for a number of applications, including, but not limited to, the visualization, identification and characterization of various active sites of BACE, and the BACE/APP inhibitor peptide complex, including the APP binding site. The active site structures may then be used to design various agents which interact with BACE, as well as BACE complexed with an APP protein or peptide, or related molecules.

[0005] The present invention is also directed to an active site of an APP binding protein or peptide, and preferably the APP peptide binding site of BACE that is elucidated and derived from the three dimensional structure of BACE as defined by the relative structural coordinates set forth in Figure 1, \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

In one embodiment of the present invention, the active site of the APP binding protein or peptide, preferably the APP peptide binding site of BACE, comprises the relative structural coordinates according to Figure 1 of residues SER71, GLY72, LEU91, ASP93, GLY95, SER96, VAL130, PRO131, TYR132, THR133, GLN134, ILE171, ILE179, ILE187, ALA188, ARG189, PRO190, TRP258, TYR259, ASP284, LYS285, ASP289, GLY291, THR292, THR293, ASN294, ARG296 and ARG368, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

[0007] In another embodiment, the active site of the APP binding protein or peptide, preferably the APP peptide binding site of BACE, comprises the

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relative structural coordinates according to Figure 1 of residues LYS70, SER71, GLY72, GLN73, GLY74, TYR75, LEU91, VAL92, ASP93, THR94, GLY95, SER96, SER97, ASN98, TYR129, VAL130, PRO131, TYR132, THR133, GLN134, GLY135, LYS136, TRP137, LYS168, PHE169, PHE170, ILE171, ASN172, SER174, TRP176, GLY178, ILE179, LEU180, GLY181, ALA183, TYR184, ALA185, GLU186, ILE187, ALA188, ARG189, PRO190, ASP191, ASP192, ARG256, TRP258, TYR259, TYR283, ASP284, LYS285, SER286, ILE287, VAL288, ASP289, SER290, GLY291, THR292, THR293, ASN294, LEU295, ARG296, GLY325, GLU326, ARG368, VAL370, LYS382, PHE383, ALA384, ILE385, SER386, GLN387, SER388, SER389, THR390, GLY391, THR392, VAL393, GLY395, ALA396 and ILE447, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

[0008] The present invention further provides a method for identifying an agent that interacts with an active site of BACE. The method comprises the steps of: (a) determining a putative active site of BACE from a three dimensional model of BACE using the relative structural coordinates of Figure 1, \pm a root mean square deviation from the backbone atoms of the amino acids of not more than 1.5Å; and (b) performing various computer fitting analyses to identify an agent which interacts with the putative active site.

I 0009] The present invention also provides method for identifying an agent that interacts with an active site of an APP binding protein or peptide, preferably BACE. The method comprises the steps of: (a) generating a three dimensional model of an active site of an APP binding protein or peptide using the relative structural coordinates according to Figure 1 of residues SER71, GLY72, LEU91, ASP93, GLY95, SER96, VAL130, PRO131, TYR132, THR133, GLN134, ILE171, ILE179, ILE187, ALA188, ARG189, PRO190, TRP258, TYR259, ASP284, LYS285, ASP289, GLY291, THR292, THR293, ASN294, ARG296 and ARG368, \pm a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å; and (b) designing an agent using the three dimensional model generated in step (a).

The present invention also provides another method for [0010] identifying an agent that interacts with an active site of an APP binding protein or peptide, preferably BACE. The method comprises the steps of: (a) generating a three dimensional model of an active site of an APP binding protein or peptide using the relative structural coordinates according to Figure 1 of residues LYS70, SER71, GLY72, GLN73, GLY74, TYR75, LEU91, VAL92, ASP93, THR94, GLY95, SER96, SER97, ASN98, TYR129, VAL130, PRO131, TYR132, THR133, GLN134, GLY135, LYS136, TRP137, LYS168, PHE169, PHE170, ILE171, ASN172, SER174, TRP176, GLY178, ILE179, LEU180, GLY181, ALA183, TYR184, ALA185, GLU186, ILE187, ALA188, ARG189, PRO190, ASP191, ASP192, ARG256, TRP258, TYR259, TYR283, ASP284, LYS285, SER286, ILE287, VAL288, ASP289, SER290, GLY291, THR292, THR293, ASN294, LEU295, ARG296, GLY325, GLU326, ARG368, VAL370, LYS382, PHE383, ALA384, ILE385, SER386, GLN387, SER388, SER389, THR390, GLY391, THR392, VAL393, GLY395, ALA396 and ILE447, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å; and (b) designing an agent using the three dimensional model generated in step (a).

[0011] Finally, the present invention provides agents, and preferably inhibitors, identified using the foregoing methods. Small molecules or other agents which inhibit or otherwise interfere with the ability of BACE to cleave APP may be useful in the treatment and/or prevention of Alzheimer's Disease.

[**0012**] Additional objects of the present invention will be apparent from the description which follows.

Brief Description of the Figure

[0013] Figure 1 provides the atomic structural coordinates for BACE and the APP inhibitor peptide as derived by X-ray diffraction of a crystal of the BACE and APP inhibitor peptide complex. "Atom type" refers to the atom whose coordinates are being measured. "Residue" refers to the type of residue of which each measured atom is a part - i.e., amino acid, cofactor, ligand or solvent. The

"x, y and z" coordinates indicate the Cartesian coordinates of each measured atom's location in the unit cell (\mathring{A}). "Occ" indicates the occupancy factor. "B" indicates the "B-value", which is a measure of how mobile the atom is in the atomic structure (\mathring{A}^2).

Detailed Description of the Invention

[0014] As used herein, the following terms and phrases shall have the meanings set forth below:

In the β-secretase enzyme that cleaves β-amyloid precursor protein (APP) at residue 671 (770aa isoform of APP numbering). After cleavage of APP by BACE, the remaining APP is cleaved at residue 716 by γ-secretase, leaving a 42 amino acid fragment of APP that is found in the proteinaceous plaques of Alzheimer's patients. The amino acid sequence of BACE preferably has the amino acid sequence deposited with Swiss Prot under accession number P56817, including conservative substitutions. As used herein, BACE also includes "BACE peptides," which are molecules having less than the complete amino acid sequence of BACE. Preferably, BACE peptides include the active site in which BACE binds to and cleaves APP. Most preferably, the BACE peptide corresponds to amino acid residues 58-447 set forth in Figure 1 ("BACE₅₈₋₄₄₇"), including conservative substitutions.

[0016] "APP" is β -amyloid precursor protein having the amino acid sequence deposited with Swiss Prot under accession number CAA31830, including conservative substitutions. As used herein, APP also includes "APP peptides," which are molecules having less than the complete amino acid sequence of APP. Preferably, APP peptides include the active site in which APP is cleaved by BACE.

[0017] An "APP inhibitor peptide" is a peptide which inhibits binding between BACE and APP. Preferably, the APP peptide has the amino acid sequence SER-GLU-VAL-ASN-Sta-VAL-ALA-GLU-PHE, where Sta is rare amino acid (S)-Statine.

[**0018**] An "APP binding protein or peptide" is a protein or peptide that binds APP and has a APP binding site, and includes but is not limited to BACE and BACE peptides.

[**0019**] Unless otherwise indicated, "protein" shall include a protein, protein domain, polypeptide or peptide.

[0020] "Structural coordinates" are the Cartesian coordinates corresponding to an atom's spatial relationship to other atoms in a molecule or molecular complex. Structural coordinates may be obtained using x-ray crystallography techniques or NMR techniques, or may be derived using molecular replacement analysis or homology modeling. Various software programs allow for the graphical representation of a set of structural coordinates to obtain a three dimensional representation of a molecule or molecular complex. The structural coordinates of the present invention may be modified from the original set provided in Figure 1 by mathematical manipulation, such as by inversion or integer additions or subtractions. As such, it is recognized that the structural coordinates of the present invention are relative, and are in no way specifically limited by the actual x, y, z coordinates of Figure 1.

[**0021**] An "agent" shall include a protein, polypeptide, peptide, nucleic acid, including DNA or RNA, molecule, compound or drug.

[**0022**] "Root mean square deviation" is the square root of the arithmetic mean of the squares of the deviations from the mean, and is a way of expressing deviation or variation from the structural coordinates of BACE described herein. The present invention includes all embodiments comprising conservative substitutions of the noted amino acid residues resulting in same structural coordinates within the stated root mean square deviation.

[0023] The numbering of the amino acid residues identified in Figure 1 are based on the numbering of the full length BACE protein from the start of the signal sequence. It will be obvious to the skilled practitioner that the numbering of the amino acid residues of BACE may be different than that set forth herein or may contain certain conservative amino acid substitutions that yield the same

three dimensional structures as those defined in Figure 1. Corresponding amino acids and conservative substitutions in other isoforms or analogues are easily identified by visual inspection of the relevant amino acid sequences or by using commercially available homology software programs (e.g., MODELLAR, MSI, San Diego, CA).

[0024] "Conservative substitutions" are those amino acid substitutions which are functionally equivalent to the substituted amino acid residue, either by way of having similar polarity, steric arrangement, or by belonging to the same class as the substituted residue (e.g., hydrophobic, acidic or basic) and includes substitutions having an inconsequential effect on the three dimensional structure of BACE, with respect to the use of this structure for the identification and design of agents which interact with BACE, for molecular replacement analyses and/or for homology modeling.

[0025] As used herein, an "active site" refers to a region of a molecule or molecular complex that, as a result of its shape and charge potential, favorably interacts or associates with another agent (including, without limitation, a protein, polypeptide, peptide, nucleic acid, including DNA or RNA, molecule, compound, antibiotic or drug) via various covalent and/or non-covalent binding forces. Preferably, the active site of BACE corresponds to the site in which BACE cleaves the APP molecule.

I 0026] As such, the active site of BACE may include, for example, both the actual site in which BACE binds and cleaves APP, as well as accessory binding sites adjacent or proximal to the actual binding site that nonetheless may affect the ability of BACE to bind and cleave APP, either by direct interference with the actual site of binding or by indirectly affecting the steric conformation or charge potential of the BACE molecule and thereby preventing or reducing the ability of BACE to bind to APP at the actual binding site. As used herein, an active site also includes BACE or BACE analog residues which exhibit observable NMR perturbations in the presence of a binding ligand, such as APP or an APP peptide. While such residues exhibiting observable NMR perturbations may not necessarily be in direct contact with or immediately

proximate to ligand binding residues, they may be critical to BACE residues for rational drug design protocols.

[**0027**] The present invention is directed to a crystallized complex of BACE and an APP inhibitor peptide that effectively diffracts X-rays for the determination of the structural coordinates of the complex. As used herein, BACE preferably corresponds to BACE₅₈₋₄₄₇ as set forth in Figure 1, with the N-terminal domain consisting of amino acid residues 58-207 shown in Figure 1, and the C-terminal domain consisting of amino acid residues 208-447 shown in Figure 1. The APP inhibitor peptide is preferably SER-GLU-VAL-ASN-Sta-VAL-ALA-GLU-PHE.

[0028] Using the crystal complex of the present invention, X-ray diffraction data can be collected by a variety of means in order to obtain the atomic coordinates of the crystallized molecule or molecular complex. With the aid of specifically designed computer software, such crystallographic data can be used to generate a three dimensional structure of the molecule or molecular complex. Various methods used to generate and refine the three dimensional structure of a crystallized molecule or molecular structure are well known to those skilled in the art, and include, without limitation, multiwavelength anomalous dispersion (MAD), multiple isomorphous replacement, reciprocal space solvent flattening, molecular replacement, and single isomorphous replacement with anomalous scattering (SIRAS).

[0029] Accordingly, the present invention also provides the three dimensional structure of BACE as derived by x-ray diffraction data of the BACE/APP inhibitor peptide crystal. Specifically, the three dimensional structure of BACE is defined by the structural coordinates shown in Figure 1, ± a root mean square deviation from the backbone atoms of the amino acids of not more than 1.5Å, preferably not more than 1.0Å, and most preferably not more than 0.5Å. The structural coordinates of BACE are useful for a number of applications, including, but not limited to, the visualization, identification and characterization of various active sites of BACE, and the BACE/APP inhibitor peptide complex, including the APP or APP peptide binding site. The active site

structures may then be used to design agents with interact with BACE, as well as BACE complexed with APP, an APP peptide or related molecules.

[0030] The present invention is also directed to an active site of an APP binding protein or peptide, preferably the APP peptide binding site of BACE, which comprises the relative structural coordinates according to Figure 1 of residues SER71, GLY72, LEU91, ASP93, GLY95, SER96, VAL130, PRO131, TYR132, THR133, GLN134, ILE171, ILE179, ILE187, ALA188, ARG189, PRO190, TRP258, TYR259, ASP284, LYS285, ASP289, GLY291, THR292, THR293, ASN294, ARG296 and ARG368, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å, more preferably not more than 1.0Å, and most preferably not more than 0.5Å.

In another preferred embodiment, the active site of an APP [0031]binding protein or peptide, preferably the APP peptide binding site of BACE, comprises the relative structural coordinates according to Figure 1 of residues LYS70, SER71, GLY72, GLN73, GLY74, TYR75, LEU91, VAL92, ASP93, THR94, GLY95, SER96, SER97, ASN98, TYR129, VAL130, PRO131, TYR132, THR133, GLN134, GLY135, LYS136, TRP137, LYS168, PHE169, PHE170, ILE171, ASN172, SER174, TRP176, GLY178, ILE179, LEU180, GLY181, ALA183, TYR184, ALA185, GLU186, ILE187, ALA188, ARG189, PRO190, ASP191, ASP192, ARG256, TRP258, TYR259, TYR283, ASP284, LYS285, SER286, ILE287, VAL288, ASP289, SER290, GLY291, THR292, THR293, ASN294, LEU295, ARG296, GLY325, GLU326, ARG368, VAL370, LYS382, PHE383, ALA384, ILE385, SER386, GLN387, SER388, SER389, THR390, GLY391, THR392, VAL393, GLY395, ALA396 and ILE447, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å, more preferably not more than 1.0Å, and most preferably not more than 0.5Å. Another aspect of the present invention is directed to a method for [0032]identifying an agent that interacts with an active site of BACE comprising the steps of: (a) determining an active site of BACE from a three dimensional model of BACE using the relative structural coordinates of Figure 1, \pm a root mean square deviation from the backbone atoms of said amino acids of not more than

1.5Å, more preferably not more than 1.0Å, and most preferably not more than 0.5Å; and (b) performing computer fitting analysis to identify an agent which interacts with said active site. Computer fitting analyses utilize various computer software programs that evaluate the "fit" between the putative active site and the identified agent, by (a) generating a three dimensional model of the putative active site of a molecule or molecular complex using homology modeling or the atomic structural coordinates of the active site, and (b) determining the degree of association between the putative active site and the identified agent. Three dimensional models of the putative active site may be generated using any one of a number of methods known in the art, and include, but are not limited to, homology modeling as well as computer analysis of raw data generated using crystallographic or spectroscopy data. Computer programs used to generate such three dimensional models and/or perform the necessary fitting analyses include, but are not limited to: GRID (Oxford University, Oxford, UK), MCSS (Molecular Simulations, San Diego, CA), AUTODOCK (Scripps Research Institute, La Jolla, CA), DOCK (University of California, San Francisco, CA), Flo99 (Thistlesoft, Morris Township, NJ), Ludi (Molecular Simulations, San Diego, CA), QUANTA (Molecular Simulations, San Diego, CA), Insight (Molecular Simulations, San Diego, CA), SYBYL (TRIPOS, Inc., St. Louis. MO) and LEAPFROG (TRIPOS, Inc., St. Louis, MO).

[0033] The present invention also provides a method for identifying an agent that interacts with an active site of an APP binding protein or peptide, and preferably the APP peptide binding site on BACE. The method comprises the steps of: (a) generating a three dimensional model of an active site of an APP binding protein or peptide using the relative structural coordinates according to Figure 1 of residues SER71, GLY72, LEU91, ASP93, GLY95, SER96, VAL130, PRO131, TYR132, THR133, GLN134, ILE171, ILE179, ILE187, ALA188, ARG189, PRO190, TRP258, TYR259, ASP284, LYS285, ASP289, GLY291, THR292, THR293, ASN294, ARG296 and ARG368, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å, more preferably not more than 1.0Å, and most preferably not more than 0.5Å;

and (b) designing an agent using the three dimensional model generated in step (a). In another preferred embodiment, the active site of the APP binding protein or peptide is generated using the three dimensional model defined by the relative structural coordinates according to Figure 1 of residues LYS70, SER71, GLY72, GLN73, GLY74, TYR75, LEU91, VAL92, ASP93, THR94, GLY95, SER96, SER97, ASN98, TYR129, VAL130, PRO131, TYR132, THR133, GLN134, GLY135, LYS136, TRP137, LYS168, PHE169, PHE170, ILE171, ASN172, SER174, TRP176, GLY178, ILE179, LEU180, GLY181, ALA183, TYR184, ALA185, GLU186, ILE187, ALA188, ARG189, PRO190, ASP191, ASP192, ARG256, TRP258, TYR259, TYR283, ASP284, LYS285, SER286, ILE287, VAL288, ASP289, SER290, GLY291, THR292, THR293, ASN294, LEU295, ARG296, GLY325, GLU326, ARG368, VAL370, LYS382, PHE383, ALA384, ILE385, SER386, GLN387, SER388, SER389, THR390, GLY391, THR392, VAL393, GLY395, ALA396 and ILE447, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å, more preferably not more than 1.0Å, and most preferably not more than 0.5Å.

The effect of such an agent identified by computer fitting analyses [0034]on the APP binding protein or peptide may be further evaluated by obtaining or synthesizing the agent, and contacting the identified agent with the APP binding protein or peptide in order to determine the effect the agent has on the APP binding protein or peptide. Preferably, the APP binding protein or peptide is BACE (or a BACE peptide), and the agent is a potential inhibitor of binding between BACE (or a BACE peptide) and APP (or an APP peptide). Therefore, in the preferred embodiment, the agent is contacted with BACE (or a BACE peptide) in the presence of APP (or a APP peptide), to determine the ability of the agent to inhibit binding between BACE (or the BACE peptide) and APP (or the APP peptide). Depending upon the action of the agent on the active site, the agent may act either as an inhibitor or activator of the BACE/APP binding. Assays may be performed and the results analyzed to determine whether the agent is an inhibitor (i.e., the agent may reduce or prevent binding affinity between BACE and APP), an activator (i.e., the agent may increase binding

affinity between BACE and APP), or has no effect on the interaction between BACE and APP. Agents identified using the foregoing methods, and preferably inhibitors of BACE cleavage of APP, may then be tested as therapeutics in the treatment and/or prevention of Alzheimer's Disease, and other diseases that are also characterized by the presence of the 42 amino acid fragment of APP in the proteinaceous plaques of the brain.

[0035] Various molecular analysis and rational drug design techniques are further disclosed in U.S. Patent Nos. 5,834,228, 5,939,528 and 5,865,116, as well as in PCT Application No. PCT/US98/16879, published WO 99/09148, the contents of which are hereby incorporated by reference.

[0036] Finally, the present invention is also directed to the agents, and preferably the inhibitors, identified using the foregoing methods. Such agents may be a protein, polypeptide, peptide, nucleic acid, including DNA or RNA, molecule, compound, or drug, and preferably are small molecules that effectively inhibit binding between BACE and APP or an APP peptide. Such molecules may be useful in treating, preventing or inhibiting progression of Alzheimer's Disease.

[0037] The present invention may be better understood by reference to the following non-limiting Example. The following Example is presented in order to more fully illustrate the preferred embodiments of the invention, and should in no way be construed as limiting the scope of the present invention.

Example 1

A. Methods

[0038] Cloning of Human BACE1. Human polyA+ mRNA from whole brain (Clontech) was converted to cDNA by random-priming using Thermoscript RT-PCR System, according to the manufacturer's protocol (Lifetechnologies). This cDNA was amplified by PCR using the forward and reverse primers, 5' GCTCTAGAACCCAGC ACGGCATCCGGCTG 3' (XbaI site indicated by underlined sequence; nts. 517-537 in accession no. AF190725) and 5' CCAAGCATGCGGCCGCAATAGGCTATGGTCA TGAGGGTTGAC 3' (NotI site

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indicated by underlined sequence; nts. 1809-1833; bold "A" indicates additional nucleotide to permit in-frame translation of the Fc chimera; see below), respectively. PCR was accomplished using Expand Long Polymerase kit according to the manufacturer's conditions (Roche Biochemicals; buffer #3), with PCR cycling consisting of an initial denaturing step at 95°C for 3min, 30-40 cycles of denaturation at 94°C for 30sec, annealing at 65°C for 30sec, elongation at 68°C for 1min 30sec, followed by a final elongation at 68°C for 5min. The PCR products were run on a 1% agarose gel. The appropriate band was cut out of the gel, purified by Quantum Prep Freeze 'N Squeeze DNA Extraction Columns (Bio-Rad), and cloned into the SpeI/NotI sites of the mammalian expression vector, pED/Fc (Kaufman, RJ et al., 1991, Nucl. Acids. Res. 19:4485-4490).

[0039] An intermediate construct contained the honey bee meletin secretory leader fused to the the prodomain and coding region of BACE1, just upstream to the predicted transmembrane domain of BACE1 (Vassar, R. et al., 1999, Science 286:735-741). The absence of the predicted hydrophobic transmembrane domain in this construct would permit soluble secreted BACE.Fc protein to be extracted from the conditioned medium. Downstream of BACE1 was an engineered enterokinase cleavage site followed by sequence encoding the Fc portion of immunoglobulin IgG. The final construct contained the BACE1.Fc gene, flanked by SalI and EcoRI in pED/Fc, cloned into the SalI/EcoRI sites of the mammalian expression vector, pHTop, a derivative of pED, in which the majority of the adenovirus major late promoter was replaced by six repeats of a bacterial tetracycline operator (described in Gossen et al, 1992, PNAS, 89:5547-5551). Sequencing of the BACE1.Fc recombinant gene was accomplished by BigDye terminator dideoxy sequencing using an ABI3700. Sequence analyses was accomplished using DNAstar software package.

I 0040] Expression of Human BACE1. The vector, pHTOP, with the BACE1.Fc insert, contains the dihydrofolate reductase gene and when introduced in the cell line CHO/A2 (see description below) functions very

efficiently and high expressers can be selected by isolating cells surviving in high methotrexate concentrations. The CHO/A2 cell line is derived from CHO DUKX B11 (Urlaub and Chasin, 1980, PNAS USA 77:4216-4220) by stably integrating a transcriptional activator (tTA), a fusion protein between the Tet repressor and the herpes virus VP16 transcriptional domain (Gossen et al). A CHO cell line expressing extracellular BACE1.Fc was established by transfecting (lipofection) pHTopBACE1.Fc into CHO/A2 cells and selecting clones in 0.02 and 0.05 µM methotrexate. The conditioned media from multiple clones were screened by Western blot using a (mouse) anti-human IgG.Fc HRP antibody. The same clones were also metabolically labeled with 35 S (met/cys). The best clone, determined by virtue of its high expression, was one which resulted from 0.05 µM MTX selection and was chosen to be scaled up for roller bottle conditioned media production (4 Liters). The conditioned media was then used for purification. The expressed protein has residues 22-460 and nine extra residues at the C-terminal (an artefact from cloning and remains of the EK cleavage site).

[0041] Purification of BACE1. For the purification of BACE the 102 liters of conditioned media was used. During purification the activity of the enzyme was estimated at room temperature by continuously monitoring the fluorescent intensity for 5-10 min. at 420 nm (ext – 320 nm) Abz-Ser-Glu-Val-Asn-Leu-Asp-Ala-Glu-Phe-Arg-Dpa (Abz = Amino benzoic acid, Dpa = 9,10-diphenylanthracene) as the substrate. The reaction mixture contained 20 μ M of substrate, different amounts of enzyme in 0.5 ml of 20 mM Tris-HCl pH 8.0 and 100 mM NaCl. The concentrated material of conditioned media(1.6 l) was applied to column (2.8 x 12 cm) containing ImmunoPure Immobilized Protein A agarose (Pierce, Il, USA) equilibrated in PBS buffer. The speed of application was 2 ml/min. The column was washed with 1 litre of PBS buffer and the BACE-Fc protein was eluted by ImmunoPure IgG Elution Buffer (Pierce, Il, USA). The fractions containing protein were immediately neutralized by 1 M Tris-HCl to pH 8.0.

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[0042] The obtained protein material was treated with Enterokinase at 25°C. The ratio of BACE-Fc to Enterokinase was 3000:1 and the time of reaction was 3 hrs. The reaction was stopped by removing Enterokinase from reaction mixture by applying the protein to a column (1 x 5 cm) containing soybean trypsin inhibitor agarose (Sigma, Mo, USA) equilibrated in 20 mM Tris-HCL pH 8.0 containing 100 mM NaCl (speed was 1 ml/min). The flow through material contained BACE and cleaved Fc. Cleaved Fc was removed from BACE by flowing through a protein A column equilibrated in 20 mM Tris-HCl pH 8.0.

[0043] BACE was partially de-glycosylated using PNGase F (New England Labs., Ma, USA). 8-9 μg of PNGase was added to 1 mg of BACE and the incubation was carried at 37° C for 16 hrs. The additional 5-6 μg of PNGase was added to each mg of BACE and incubation was continued for another 4 hrs. The purified BACE was separated from PNGase by HPLC size-exclusion

elution was 3 ml/min). The purified BACE was concentrated and used for crystallization experiments.

[0044] N-terminal sequencing of purified BACE reveals a mixture of protein species, with the major sample having the processing domain cleaved and beginning at residue 47 (all numbering refers to full length BACE; accession code: A59090) and a minor sample which had not been cleaved beginning at

residue 22. A smaller sample with sequence MTIAY was also detected.

chromatography using 21.5 x 30 cm G-3000SW column (TosoHaas, Pa, USA)

equilibrated in 20 mM tris-HCL pH 8.0 containing 200 mM NaCl. (Speed of

[0045] Crystallization. The crystals were grown using the hanging drop vapour diffusion method. The protein was concentrated to mg/ml in 20mM Tris pH 7.5, 200mM sodium chloride. Inhibitor peptide sequence is SEVNStaVAEF, where Sta is the rare amino acid (S)-Statine. It was concentrated to 100mM in 100% DMSO and mixed with concentrated protein in a two-fold peptide excess to form the complex. 1 μ l of complex was added to 1 μ l of well solution containing 100mM Sodium Cacodylate pH6.5, 25% PEG8K, 300mM lithium sulphate. Plate-like crystal clusters grew within one week to dimensions of 200

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 μ m x 400 μ m x 75 μ m. Single crystals were transferred to a stabilizing, cryoprotectant solution which contained the well solution plus 25% Glycerol for a brief, 10 second, soak and then frozen in liquid nitrogen. X-ray diffraction crystals had space group I222, and unit cell parameters a=86.627, b=130.861, c=130.729, and α = β = γ =90°.

B. Results

Expressed in CHO cells as a fc fusion protein and, after purification, cleavage and partial deglycosylation, complexed with peptide inhibitor and crystallized. Crystals diffracted to 2.3Å and the structure was solved using the technique of molecular replacement. The search model used was derived from cod atlantic Pepsin and contained 63% of the final number of atoms. The density modified maps obtained using a poly-alanine version of the search model (39% of the final atoms) provided sufficient information to build all but 12 amino acids. The final model contains residues from 59 to 448 (using full length numbering), all 9 residues of the statine inhibitor and 360 water molecules. Of the four predicted N-linked glycosylation sites only two have interpretable electron density.

[0047] The overall shape of the BACE protein is spherical and is composed of two distinct domains, an N-terminal (58-207) and a C-terminal (208-447). With the first thirteen amino acids (58-71) being packed against residues 238-243. There is a significant cleft-like channel across one surface of the interface between the domains. This contains the inhibitor peptide and conserved aspartic acid motifs that define the active sites of aspartic proteases.

[0048] The N-terminal domain is composed of a single a-helix preceding the loop joining the two domains and thirteen β -strands. The larger C-terminal domain has a total of seventeen β -strands and three α -helices. The overall topology is characterised by an eight stranded antiparallel interdomain β -sheet. This central sheet comprises the majority of the active site residues including the two conserved aspartates (one from each domain:93 and 289). Asp93 and

Asp289 define the position of a pseudo two-fold axis for the central β -sheet. Outside of this symmetry the two domains differ significantly. The N-terminal domain has an extra two strands extending the central sheet. In addition, there are two anti-parallel β -sheets above and below the central sheet composed of three and four β -strands respectively. Residues from the upper sheet (131-135) fold over the active site aspartates and form a 'flap' over the centre of the peptide binding cleft.

[0049] The C-terminal domain contains two lobes in addition to the strands which from the central β -sheet. These are weakly homologous to known aspartic protease structures. The binding pocket for the P1`and P3`positions are instead derived from three β -turns 388-391, 284-286 and 255-261.

[**0050**] There are a total of six cysteine residues in BACE. Each of these is involved in a disulphide interaction. The pattern of disulphide crosslinking, Cys278-Cys443, Cys380-Cys330, Cys420-Cys216 are unique in the aspartic proteases known to date.

[0051] A novel aspartic protease. The first attempts to study the relationship of function to structure of an Apartic proteases began in the 1930s with Pepsin. Since then this rich field of research has been successfully applied to the design of clinically used inhibitors in only one system; HIV protease. The reasons for this are related more to the validity of the pharmacological target than the efficacy of inhibitors. β -secretase has been described as a novel protease and has been shown to be linked to the onset and progression of Alzheimer's disease.

[0052] From a gross viewpoint the overall fold and domain organization is very similar to that of a canonical aspartic protease. The comparison at a more detailed level reveals a significant number of differences. The active site is characterized by two aspartic residues surrounded by a conserved set of hydrogen bonds termed a 'fireman's grip'. This is reproduced in the -secretase structure presented here. The characteristic flap which wraps over the active site in pepsin is absent from the C-terminal domain in a manner analogous to

cathepsin D. In β -secretase the critical main chain amide hydrogen bond to the carboxyl group of statine is maintained by Thr133 from this flap. The amide of the statine makes a hydrogen bond to the carboxyl group of Gly95, emphasizing that the statine residue occupies both the P1 and P1` position.

Enzyme Mechanism. It has been shown that β -secretase cleavage [0053]is dependent on proximity to the cell membrane. Both β -secretase and its substrate APP have putative transmembrane regions. Our expressed BACE construct finishes one amino acid before the predicted transmembrane region. The final residue in the current structure is Ile447, thirteen residues away from the beginning of the putative transmembrane domain. In the current crystal structure Ile447 is only 6Å away from the P3 Glutamic acid of the inhibitor suggesting a role for the remaining C-terminal residues in the enzyme mechanism. The Statine residue of the inhibitor peptide is bound at the \$1 position within the active site. The position of the C-3 hydroxyl group, coplanar to and within hydrogen bonding distance of both aspartate 93 and 289 carboxyl groups, confirms that the rare amino acid mimics the tetrahedral transition state i.e the intermediate of peptide-bond hydrolysis. The distance between the oxygen atoms of Asp93 and Asp289 is 2.8Å, strongly suggesting a shared proton atom and a classic aspartic protease pK profile for these side-chains and a common enzyme mechanism to other known aspartic proteases.

[0054] Inhibitor binding. The inhibitor peptide binds in an extended form along a 20Å groove formed at the interface between the domains. The conserved catalytic aspartic residues lie at the middle of this groove. The bound peptide consists of 8 amino acids plus a statine amino acid at position 5. There is contiguous electron density for the whole peptide. The statine based inhibitor used in this study has been show to inhibit the β -secretase enzyme with nanomolar efficiency. The peptide sequence is based on the P10 to P4` APP751 Sweedish family mutation. This mutation of a Lys-Asn at the P2 position and Met-Leu at the P1 position is strongly correlated to the early onset of

Alzheimer's disease. The inhibitor peptide utilizes Statine's Leucyl like side-chain to explore this interaction. Due to the di-peptide nature of Satine the P1' position of the substrate is shifted to P2' leaving an empty S1' pocket. The β -secretase enzyme appears to have a novel preference for an apartate or glutamate at the P1' position whereas other aspartic proteases show a preference for hydrophobic residues. This unusual preference for a negatively charged P1' amino acid is explained by the guanadinium group of Arg189 forming part of the putative S1' pocket. Even at the acidic pH optima of BACE the arginine side chain would form a positively charged environment for the possibly protonated carboxyl side-chain atoms.

[0055] The S1 and S3 binding pockets are a contiguous, hydrophobic pocket formed by the side-chain of residues Tyr132, Phe169, Ile171, Trp176, Ile179 and main chain atoms of Gly74, and Gln73. This packing of inhibitor P1 and P3 side chains has been seen in previous aspartic protease complexes.

In the canonical APP cleavage site for b-secretase appears to have a preference for a small hydrophobic residues at the P2' position. The side chain of the valine residue bound in the putative S2' site of β -secretase appears to not make any significant interactions with the protein, its main chain however forms a tight set of hydrogen bonds to the backbone carboxyl of Gly 95 and the sidechain OH of Tyr259. In turn, Tyr259 is held rigidly in place by an edge-pi interaction with Trp258, which packs against the guanadinium group of Arg256.

[0057] Swedish mutation. Autosomal dominant mutations identified on the β -amyloid precusor protein have been correlated to early-onset cases of Alzheimer's disease. These have been shown to cluster around the three canonical cleavage sites. A double (the so-called Swedish) mutation of Lys670-Met671 (770aa isoform of APP numbering) to Asn-Leu causes an increase in the overall quantity of $A\beta$ detectable in the plasma and in the medium of cultured fibroblasts from carriers of the Swedish mutation. These two amino acids lie at the P2 and P1 positions of the β -secretase active site. The statine based inhibitor used here is based on this Swedish mutation. A methionine at position

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P1 would clearly be accommodated but would loose the van Der Waal's complentarity exhibited by the statine side-chain to Leu90 and Ile178. The C€ atom of the methione would make supplement the hydrophobic interaction to Phe169.

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Table 1

Residues of BACE Within 4Å of Peptide Inhibitor SER71, GLY72, LEU91, ASP93, GLY95, SER96, VAL130, PRO131, TYR132, THR133, GLN134, ILE171, ILE179, ILE187, ALA188, ARG189, PRO190, TRP258, TYR259, ASP284, LYS285, ASP289, GLY291, THR292, THR293, ASN294, ARG296, ARG368

Residues of BACE Within 8Å of Peptide Inhibitor LYS70, SER71, GLY72, GLN73, GLY74, TYR75, LEU91, VAL92, ASP93, THR94, GLY95, SER96, SER97, ASN98, TYR129, VAL130, PRO131, TYR132, THR133, GLN134, GLY135, LYS136, TRP137, LYS168, PHE169, PHE170, ILE171, ASN172, SER174, TRP176, GLY178, ILE179, LEU180, GLY181, ALA183, TYR184, ALA185, GLU186, ILE187, ALA188, ARG189, PRO190, ASP191, ASP192, ARG256, TRP258, TYR259, TYR283, ASP284, LYS285, SER286, ILE287, VAL288, ASP289, SER290, GLY291, THR292, THR293, ASN294, LEU295, ARG296, GLY325, GLU326, ARG368, VAL370, LYS382, PHE383, ALA384, ILE385, SER386, GLN387, SER388, SER389, THR390, GLY391, THR392, VAL393, GLY395, ALA396, ILE447

All publications mentioned herein above, whether to issued [0058] patents, pending applications, published articles, deposited sequences, or otherwise, are hereby incorporated by reference in their entirety. While the foregoing invention has been described in some detail for purposes of clarity and understanding, it will be appreciated by one skilled in the art from a reading of the disclosure that various changes in form and detail can be made without departing from the true scope of the invention in the appended claims.

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What is claimed is:

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1. A crystallized complex of Beta-site APP Cleaving Enzyme (BACE) and SER-GLU-VAL-ASN-Sta-VAL-ALA-GLU-PHE.

- 2. The crystallized complex of Claim 1, wherein BACE has an N-terminal domain consisting of amino acid residues 58-207 shown in Figure 1, and a C-terminal domain consisting of amino acid residues 208-447 shown in Figure 1.
- 3. An active site of an APP binding protein or peptide comprising the relative structural coordinates according to Figure 1 of residues SER71, GLY72, LEU91, ASP93, GLY95, SER96, VAL130, PRO131, TYR132, THR133, GLN134, ILE171, ILE179, ILE187, ALA188, ARG189, PRO190, TRP258, TYR259, ASP284, LYS285, ASP289, GLY291, THR292, THR293, ASN294, ARG296 and ARG368, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.
- 4. The active site of Claim 3, wherein the \pm a root mean square deviation from the backbone atoms of said amino acids is not more than 1.0Å.
- 5. The active site of Claim 3, wherein the \pm a root mean square deviation from the backbone atoms of said amino acids is not more than 0.5Å.
- 6. An active site of an APP binding protein or peptide comprising the relative structural coordinates according to Figure 1 of residues LYS70, SER71, GLY72, GLN73, GLY74, TYR75, LEU91, VAL92, ASP93, THR94, GLY95, SER96, SER97, ASN98, TYR129, VAL130, PRO131, TYR132, THR133, GLN134, GLY135, LYS136, TRP137, LYS168, PHE169, PHE170, ILE171,

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ASN172, SER174, TRP176, GLY178, ILE179, LEU180, GLY181, ALA183, TYR184, ALA185, GLU186, ILE187, ALA188, ARG189, PRO190, ASP191, ASP192, ARG256, TRP258, TYR259, TYR283, ASP284, LYS285, SER286, ILE287, VAL288, ASP289, SER290, GLY291, THR292, THR293, ASN294, LEU295, ARG296, GLY325, GLU326, ARG368, VAL370, LYS382, PHE383, ALA384, ILE385, SER386, GLN387, SER388, SER389, THR390, GLY391,

THR392, VAL393, GLY395, ALA396 and ILE447, ± a root mean square

1.0Å.

7. The active site of Claim 6, wherein the \pm a root mean square deviation from the backbone atoms of said amino acids is not more than

deviation from the backbone atoms of said amino acids of not more than 1.5Å.

- The active site of Claim 6, wherein the \pm a root mean 8. square deviation from the backbone atoms of said amino acids is not more than 0.5Å.
- 9. A method for identifying an agent that interacts with an active site of Beta-site APP Cleaving Enzyme (BACE), comprising the steps of:
- determining an active site of BACE from a three (a) dimensional model of BACE using the relative structural coordinates of Figure 1, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å; and
- (b) performing computer fitting analysis to identify an agent which interacts with said active site.
- 10. The method of Claim 9, wherein the \pm a root mean square deviation from the backbone atoms of said amino acids is not more than 1.0Å.
- The method of Claim 9, wherein the \pm a root mean square 11. deviation from the backbone atoms of said amino acids is not more than 0.5Å.

- 12. A method for identifying an agent that interacts with an active site of an APP binding protein or peptide, comprising the steps of:
- (a) generating a three dimensional model of an active site of an APP binding protein or peptide using the relative structural coordinates according to Figure 1 of residues SER71, GLY72, LEU91, ASP93, GLY95, SER96, VAL130, PRO131, TYR132, THR133, GLN134, ILE171, ILE179, ILE187, ALA188, ARG189, PRO190, TRP258, TYR259, ASP284, LYS285, ASP289, GLY291, THR292, THR293, ASN294, ARG296 and ARG368, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å; and
- (b) designing an agent using the three dimensional model generated in step (a).
- 13. The method of Claim 12, wherein the \pm a root mean square deviation from the backbone atoms of said amino acids is not more than 1.0Å.
- 14. The method of Claim 12, wherein the \pm a root mean square deviation from the backbone atoms of said amino acids is not more than 0.5Å.
- 15. The method of Claim 12, wherein the agent is designed by performing computer fitting analysis of the agent with the three dimensional model generated in step (a).
- 16. The method of Claim 12, further comprising the steps of: (c) obtaining or synthesizing the agent so designed; and (d) contacting the agent with the APP binding protein or peptide in order to determine the effect the agent has on the APP binding protein or peptide.

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- The method of Claim 12, wherein the APP binding protein 17. or peptide is BACE.
- 18. The method of Claim 17, wherein the agent is a potential inhibitor of binding between BACE and APP.
- The method of Claim 18, further comprising the steps of: 19. (c) obtaining or synthesizing the agent so designed; and (d) contacting the agent with BACE in the presence of APP.
- A method for identifying an agent that interacts with an 20. active site of an APP binding protein or peptide, comprising the steps of:
- generating a three dimensional model of an active site of (a) an APP binding protein or peptide using the relative structural coordinates according to Figure 1 of residues LYS70, SER71, GLY72, GLN73, GLY74, TYR75, LEU91, VAL92, ASP93, THR94, GLY95, SER96, SER97, ASN98, TYR129, VAL130, PRO131, TYR132, THR133, GLN134, GLY135, LYS136, TRP137, LYS168, PHE169, PHE170, ILE171, ASN172, SER174, TRP176, GLY178, ILE179, LEU180, GLY181, ALA183, TYR184, ALA185, GLU186, ILE187, ALA188, ARG189, PRO190, ASP191, ASP192, ARG256, TRP258, TYR259, TYR283, ASP284, LYS285, SER286, ILE287, VAL288, ASP289, SER290, GLY291, THR292, THR293, ASN294, LEU295, ARG296, GLY325, GLU326, ARG368, VAL370, LYS382, PHE383, ALA384, ILE385, SER386, GLN387, SER388, SER389, THR390, GLY391, THR392, VAL393, GLY395, ALA396 and ILE447, ± a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å; and
- (b) designing an agent using the three dimensional model generated in step (a).
- 21. The method of Claim 18, wherein the \pm a root mean square deviation from the backbone atoms of said amino acids is not more than 1.0Å.

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- 22. The method of Claim 20, wherein the \pm a root mean square deviation from the backbone atoms of said amino acids is not more than 0.5Å.
- 23. The method of Claim 20, wherein the agent is designed by performing computer fitting analysis of the agent with the three dimensional model generated in step (a).
- 24. The method of Claim 20, further comprising the steps of: (c) obtaining or synthesizing the agent so designed; and (d) contacting the agent with the APP binding protein or peptide in order to determine the effect the agent has on the APP binding protein or peptide.
- 25. The method of Claim 20, wherein the APP binding protein or peptide is BACE.
- 26. The method of Claim 25, wherein the agent is a potential inhibitor of binding between BACE and APP.
- 27. The method of Claim 26, further comprising the steps of: (c) obtaining or synthesizing the agent so designed; and (d) contacting the agent with BACE in the presence of APP.
 - 28. An agent identified by the method of Claim 9.
 - 29. An agent identified by the method of Claim 12.
 - 30. An agent identified by the method of Claim 20.

Figure 1

		Aton	n Res.		<u>x</u>	<u>Y</u> .	<u>z</u>	
		Туре			_	-	_	1 00 50 33
MOTA	1	1/4	GLY A	58	31.563		16.324	1.00 59.33
MOTA	2	CA	GLY A	58	32.863		16.764	1.00 58.44
ATOM	3	C	GLY A	58	33.594		17.727	1.00 57.81
ATOM	4	0	GLY A	58	34.06		17.333	1.00 56.66
MOTA	5	N	SER A	59	33.712		18.975	1.00 56.66
ATOM	6	CA	SER A	59	34.393		20.015	1.00 55.45
MOTA	7	C	SER A	59	33.560		21.293	1.00 53.77
MOTA	8	0	SER A	59	32.978		21.704	1.00 54.40
MOTA	9	CB	SER A	59	35.783		20.309	1.00 55.79
ATOM	10	OG	SER A	59	35.690		20.899	1.00 57.07
ATOM	11	N	PHE A	60	33.480		21.927	1.00 49.96
ATOM	12	CA	PHE A		32.719		23.181	1.00 45.72
ATOM	13	C	PHE A	60	33.683		24.247	1.00 44.79
MOTA	14	0	PHE A		33.499		24.831	1.00 45.45
ATOM	15	CB	PHE A		31.56		22.976	1.00 43.28
MOTA	16	CG	PHE A		30.55		21.957 20.602	1.00 41.00
MOTA	17	CD1			30.87			1.00 40.54
MOTA	18	CD2 CE1	PHE A		29.30 29.95		22.355 19.658	1.00 40.58 1.00 39.88
ATOM	19		PHE A		28.37		21.419	1.00 39.50
MOTA MOTA	20 21	CE2 CZ	PHE A		28.70		20.070	1.00 39.30
ATOM	22	N	VAL A		34.70		24.500	1.00 33.23
	23	CA	VAL A		35.76		25.483	1.00 43.29
ATOM .	23 24	CA	VAL A		35.24		26.738	1.00 43.13
ATOM	25	0	VAL A		35.87		27.247	1.00 42.54
ATOM	25 26	CB	VAL A		36.53		25.895	1.00 42.54
MOTA	20 27		VAL A		37.06		24.655	1.00 44.38
ATOM	28		VAL A		35.62		26.676	1.00 44.38
ATOM	29 29	N N	GLU A		34.11		27.252	1.00 40.86
ATOM	30	CA	GLU A		33.51		28.470	1.00 40.02
ATOM	31	C	GLU A		33.20		28.320	1.00 36.45
ATOM	32	ō	GLU A		33.36		29.301	1.00 36.49
ATOM	33	CB	GLU A		32.22		28.832	1.00 43.76
ATOM	34	CG	GLU A		32.39		29.764	1.00 48.74
ATOM	35	CD	GLU A		32.74		31.188	1.00 51.91
ATOM	36	OE1	GLU A		32.31		31.612	1.00 53.41
MOTA	37	OE2	GLU A	62	33.42	3 49.271	31.890	1.00 53.64
ATOM	38	Ŋ	MET A	63	32.78	0 45.062	27.129	1.00 30.86
ATOM	39	CA	MET A	63	32.42	1 43.643	26.896	1.00 27.79
MOTA	40	С	MET A	63	33.49	1 42.741	26.279	1.00 26.02
MOTA	41	0	MET A	63	33.35	4 41.476	26.310	1.00 25.25
MOTA	42	CB	MET A	63		0 43.578	26.078	1.00 25.63
MOTA	43	CG	MET A	63	29.94		26.858	1.00 24.89
ATOM	44	SD	MET A	63	28.39	2 44.180	25.960	1.00 23.85
ATOM	45 [.]	CE	MET A	63	28.43	1 45.848	25.316	1.00 24.18
MOTA	46	N	VAL A		34.55		25.736	1.00 23.39
ATOM	47	CA	VAL A	64	35.63		25.143	1.00 20.76
ATOM	48	С	VAL A	64	36.26	3 41.634	26.216	1.00 20.06
ATOM	49	O	VAL A		36.53		27.370	1.00 18.87
MOTA	50	CB	VAL A		36.74		24.517	1.00 21.16
ATOM	51		VAL A		37.95		24.151	1.00 18.99
ATOM	52	CG2			36.19		23.266	1.00 21.01
MOTA	53	N	ASP A		36.48		25.869	1.00 18.21
MOTA	54	CA	ASP A		37.09		26.800	1.00 18.56
ATOM	55	С	ASP A		36.28		28.071	1.00 17.80
ATOM	56	0	ASP A		36.86		29.165	1.00 16.29
ATOM	57	CB	ASP A		38.50		27.194	1.00 21.53
MOTA	58	CG	ASP A	65	39.40	9 40.055	25.993	1.00 22.65

MOTA	59	ODI	ASP	Α	65	39.162	39.451	24.930	1.00 23.75
MOTA	60	OD2	ASP	Α	65	40.375	40.831	26.117	1.00 24.72
ATOM	61	N	ASN	Α	66	34.955	39.209	27.969	1.00 16.59
ATOM	62	CA	ASN		66	34.090	38.987	29.156	1.00 16.58
						33.719	37.508	29.274	
MOTA	63		ASN		66				1.00 17.20
MOTA	64	0	ASN		66	32.815	37.125	30.070	1.00 19.23
ATOM	65	CB	ASN	Α	66	32.817	39.845	29.059	1.00 14.62
ATOM	66	CG	ASN	Α	66	31.967	39.516	27.835	1.00 15.57
ATOM	67		ASN		66	32.381	38.714	26.937	1.00 16.31
						30.788			
MOTA	68		ASN		66		40.120	27.760	1.00 14.85
MOTA	69	N	LEU		67 ·	34.409	36.664	28.515	1.00 17.73
MOTA	70	CA	LEU	Α	67	34.134	35.206	28.529	1.00 17.36
MOTA	71	С	LEU	A	67	35.295	34.328	28.985	1.00 16.04
MOTA	72	0	LEU	Α	67	36.499	34.701	28.842	1.00 16.38
ATOM	73	СВ	LEU		67	33.707	34.757	27.128	1.00 17.19
ATOM	74	CG	LEU		67	32.226	34.504	26.839	1.00 18.63
ATOM	75		LEU		67	31.349	35.604	27.407	1.00 16.94
ATOM	76	CD2	LEU	Α	67	32.049	34.375	25.330	1.00 18.67
ATOM	77	N	ARG	Α	68	34.956	33.166	29.531	1.00 14.58
ATOM	78	CA	ARG	Α	68	35.961	32.173	29.973	1.00 16.73
ATOM	79	C	ARG		68	35.394	30.775	29.717	1.00 15.78
MOTA	80	0	ARG		68	34.154	30.610	29.500	1.00 13.85
ATOM	81	CB	ARG	Α	68	36.299	32.349	31.459	1.00 18.19
MOTA	82	CG	ARG	Α	68	37.086	33.623	31.766	1.00 21.67
MOTA	83.	CD	ARG	Α	68	37.571	33.646	33.213	1.00 23.25
MOTA	84	NE	ARG	Α	68	36.462	33.653	34.165	1.00 26.34
ATOM	85	CZ	ARG		68	36.598	33.500	35.482	1.00 27.29
MOTA	86	•	ARG		68	37.802	33.324		1.00 25.91
MOTA	87		ARG		68	35.530	33.527	36.271	1.00 26.77
MOTA	88	N	GLY		69	36.262	29.769	29.726	1.00 14.89
MOTA	89	CA	GLY	Α	69	35.816	28.409	29.486	1.00 15.62
MOTA	90	С	GLY	A	69	36.505	27.806	28.277	1.00 16.66
MOTA	91	0	GLY	Α	69	37.526	28.367	27.771	1.00 15.60
ATOM	92	N	LYS		70	35.989	26.676	27.804	1.00 17.25
MOTA	93	CA	LYS		70	36.556	25.973	26.629	1.00 16.95
MOTA	94	С	LYS		70	35.472	25.138	25.949	1.00 16.87
ATOM	95	0	LYS		70	34.394·	24.864	26.562	1.00 17.19
MOTA	96	CB	LYS	A	70	37.737	25.092	27.058	1.00 18.62
MOTA	97	CG	LYS	Α	70	37.518	24.303	28.348	1.00 19.97
ATOM	98	CD	LYS	A	70	38.737	23.446	28.667	1.00 22.43
ATOM	99	CE	LYS		70	38.538	22.611	29.926	1.00 23.77
ATOM	100	NZ	LYS		70	39.660	21.638	30.129	1.00 22.43
	101	N			71	35.714	24.729	24.706	1.00 15.11
ATOM			SER						
ATOM	102	CA	SER		71	34.706	23.950	23.940	1.00 14.34
MOTA	103	С	SER	Α	71	34.155	22.730	24.667	1.00 14.36
ATOM	104	0	SER	Α	71	32.918	22.446	24.600	1.00 13.81
ATOM	105	CB	SER	Α	71	35.281	23.523	22.581	1.00 14.97
MOTA	106	OG	SER		71	36.456	22.743	22.732	1.00 15.41
ATOM	107	N	GLY		72	35.024	22.005	25.362	1.00 14.38
							20.815		
ATOM	108	CA	GLY		72	34.588		26.072	1.00 14.63
ATOM	109	С	GLY		72	33.661	21.022	27.262	1.00 16.49
MOTA	110	0	GLY	Α	72	32.772	20.159	27.537	1.00 16.20
MOTA	111	N	GLN	A.	73	33.814	22.129	27.979	1.00 16.78
ATOM	112	CA	GLN		73	32.965	22.369	29.167	1.00 18.67
ATOM	113	C	GLN		73	32.040	23.570	29.038	1.00 18.70
	114	O,			73 73		23.858	29.967	1.00 19.81
MOTA			GLN			31.223			
ATOM	115	CB	GLN		73	33.852	22.522	30.401	1.00 20.09
ATOM	116	CG	GLN		73	34.924	21.433	30.493	1.00 24.21
MOTA	117	CD	GLN		73	35.624	21.400	31.837	1.00 24.83
MOTA	118	OE1	GLN	A	73	36.048	22.467	32.380	1.00 26.53
MOTA	119	NE2	GLN		73	35.769	20.206	32.395	1.00 25.73
ATOM	120	N	GLY		74	32.138	24.274	27.914	1.00 17.65
*** 011	220	-•	111	4.5	, -2	JE-130	22,217	& , . J _ T	2.00 27.00

MOTA	121	CA	GLY A	74	31.292	25.429	27.688	1.00 15.83
MOTA	122	С	GLY A	74	31.939	26.746	28.068	1.00 15.56
MOTA	123	0	GLY A	74	32.837	26.799	28.962	1.00 17.53
ATOM	124	N	TYR A	. 75	31.517	27.814	27.403	1.00 13.96
ATOM	125	CA	TYR A			29.164	27.686	1.00 16.12
ATOM	126	C	TYR A			29.903	28.502	
ATOM	127	0	TYR A			29.793	28.217	1.00 14.71
MOTA	128	CB	TYR A			29.918	26.385	1.00 17.79
MOTA	129	CG	TYR A	A 75	33.490	29.354	25.605	1.00 18.92
MOTA	130	CD1	TYR A	3 . 75	33.326	28.271	24.742	1.00 19.83
MOTA	131	CD2	TYR A	A 75	34.763	29.909	25.735	1.00 20.43
MOTA	132	CE1	TYR A	75	34.409	27.757	24.020	1.00 21.98
MOTA	133	CE2	TYR A	A 75	35.847	29.407	25.025	1.00 21.04
ATOM	134	CZ	TYR A		= = : : : :	28.339	24.170	1.00 22.04
MOTA	135	OH	TYR A			27.882	23.456	1.00 22.86
ATOM	136	N	TYR A					
						30.653	29.507	1.00 13.66
ATOM	137	CA	TYR A			31.360	30.368	1.00 12.95
ATOM	138	C	TYR A			32.837	30.593	1.00 13.47
MOTA	139	0	TYR A			33.345	30.391	1.00 13.77
MOTA	140	CB	TYR A	A 76		30.662	31.725	1.00 13.31
ATOM	141	CG	TYR A	A 76	31.723	30.548	32.446	1.00 14.55
ATOM	142	CD1	TYR A	A 76	32.601	29.497	32.174	1.00 16.16
ATOM	143	CD2	TYR A	A 76	32.105	31.495	33.392	1.00 15.68
ATOM	144	CE1	TYR A	A 76	33.829	29.392	32.832	1.00 17.64
MOTA	145	CE2	TYR A			31.402	34.055	1.00 18.14
ATOM	146	CZ	TYR A			30.348	33.770	1.00 18.24
MOTA	147	OH	TYR A			30.252	34.428	1.00 21.79
	148							
MOTA		N	VAL A			33.546	31.017	1.00 12.55
ATOM	149	CA	VAL A		•	34.980	31.298	1.00 14.17
ATOM	150	C	VAL A			35.225	32.727	1.00 15.16
ATOM	151	0	VAL A			34.439	33.283	1.00 16.09
ATOM	152		VAL A			35.821	30.336	1.00 13.43
ATOM	153		VAL A			35.528	30.567	1.00 11.59
ATOM	154		VAL A			37.305	30.524	1.00 10.74
ATOM	155	N	GLU A		29.905	36.276	33.352	1.00 16.88
ATOM	156	CA	GLU A		29.486	36.571	34.731	1.00 17.45
ATOM	157	С	GLU A	A 78	28.178	37.345	34.706	1.00 16.89
ATOM	158	0	GLU A	A 78	27.961	38.239	33.826	1.00 14.65
MOTA	159	CB	GLU A	A 78	30.538	37.392	35.479	1.00 19.11
MOTA	160	CG	GLU A	A 78	30.222	37.503	36.974	1.00 24.70
MOTA	161	CD	GLU A	A 78	31.225	38.342	37.757	1.00 26.24
MOTA	162	OE1	GLU A	A 78		39.584	37.679	1.00 27.53
MOTA	163	OE2	GLU A	A 78		37.755	38.452	1.00 29.49
ATOM	164	N	MET 2			37.012	35.641	1.00 16.65
MOTA	165	CA	MET A			37.684	35.761	1.00 17.22
ATOM	166	C .	MET A			37.768	37.232	1.00 17.77
ATOM	167	ō	MET A			37.066	38.100	1.00 18.29
ATOM	168	СВ	MET A			36.899	35.007	
ATOM	169	CG	MET A			36.874	33.492	1.00 16.88
ATOM	170	SD	MET A					1.00 16.65
MOTA	171	CE				35.865	32.673	1.00 17.43
			MET A			37.003	32.577	1.00 15.55
ATOM	172	N	THR A			38.617	37.539	1.00 17.73
ATOM	173	CA	THR A			38.741	38.917	1.00 17.50
MOTA	174	C	THR A			38.630	38.853	1.00 17.85
MOTA	175	0	THR A			39.075	37.851	1.00 17.14
MOTA	176	CB	THR A			40.100	39.550	1.00 18.12
MOTA	177	OG1				41.158	38.857	1.00 18.55
MOTA	178	CG2				40.328	39.474	1.00 16.48
MOTA	179	N	VAL A			38.020	39.874	1.00 18.24
ATOM	180	CA	VAL 2			37.882	39.959	1.00 20.23
MOTA	181	С	VAL A			38.274	41.375	1.00 21.18
ATOM	182	0	VAL A	A 81	20.929	38.093	42.362	1.00 20.31

MOTA	183	CB	VAL	A	81	20.105	36.429	39.700	1.00 20.43
ATOM	184	CG1	VAL	Α	81	20.566	35.959	38.334	1.00 21.49
MOTA	185	CG2	VAL	Δ	81	20.639	35.518	40.777	1.00 21.78
MOTA	186	И	GLY		82	18.938	38.817	41.497	1.00 21.84
MOTA	187	CA	·GLY	A	82	18.421	39.200	42.799	1.00 21.10
ATOM	188	С	GLY	Α	82	18.973	40.475	43.404	1.00 21.47
	189	Ō	GLY		82	19.864			
MOTA							41.159	42.814	1.00 21.97
ATOM	190	N	SER	A	83	18.454	40.808	44.581	1.00 22.27
MOTA	191	CA	SER	Α	83	18.869	42.012	45.335	1.00 22.02
MOTA	192	С	SER		83	18.996	41.607	46.795	1.00 20.16
MOTA	193	О	SER		83	18.002	41.120	47.410	1.00 20.07
MOTA	194	CB	SER	Α	83	17.804	43.104	45.213	1.00 21.98
MOTA	195	OG	SER	Δ	83	17.356	43.229	43.874	1.00 23.70
MOTA	196	N	PRO		84	20.198	41.734	47.380	1.00 21.14
MOTA	197	CA	PRO	A.	84	21.454	42.221	46.785	1.00 20.45
MOTA	198	С	PRO	Α	84	21.911	41.288	45.656	1.00 20.37
MOTA	199	0	PRO		84	21.508	40.086	45.606	1.00 18.46
MOTA	200	CB	PRO		84	22.434	42.193	47.962	1.00 19.74
ATOM	201	CG	PRO	Α	84	21.548	42.320	49.166	1.00 20.71
ATOM	202	CD	PRO	Ά	84	20.377	41.447	48.815	1.00 19.44
	203								
MOTA		N	PRO		85	22.754	41.790	44.741	1.00 20.53
MOTA	204	CA	PRO	Α	85 ·	23.258	40.997	43.616	1.00 20.58
ATOM	205	С	PRO	Α	85	23.949	39.706	44.046	1.00 20.81
ATOM	206	0	PRO	Δ	85	24.854	39.720	44.936	1.00 21.15
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MOTA	207	CB	PRO		85	24.240	41.947	42.932	1.00 20.87
MOTA	208	CG	PRO	Α	85	23.732	43.294	43.282	1.00 22.23
ATOM	209	CD	PRO	Α	85	23.340	43.141	44.724	1.00 21.41
ATOM	210	N	GLN		86	23.541	38.590	43.453	1.00 20.05
MOTA	211	CA	GLN		86	24.174	37.289	43.752	1.00 19.63
MOTA	212	С	GLN	Α	86	24.904	36.923	42.472	1.00 20.50
ATOM	213	0	GLN	Α	86	24.263	36.622	41.412	1.00 19.85
ATOM	214	СВ	GLN		86	23.127	36.227		
								44.097	1.00 19.82
MOTA	215	CG	GLN	A	86	22.283	36.586	45.314	1.00 18.97
MOTA	216	CD	GLN	Α	86	21.292	35.506	45.693	1.00 19.84
ATOM	217	OE1	GLN	Α	86	20.226	35.801	46.316	1.00 21.21
ATOM	218	NE2			86				
						21.603	34.259	45.354	1.00 17.54
ATOM	219	N	THR		87	26.229	36.969	42.527	1.00 19.61
MOTA	220	CA	THR	Α	87	27.057	36.669	41.346	1.00 19.61
MOTA	221	С	THR	Α	87	27.088	35.188	40.994	1.00 18.63
MOTA	222	ō	THR		87	27.220	34.302	41.892	1.00 18.56
MOTA	223	CB	THR		87	28.501	37.164	41.549	1.00 19.88
MOTA	224	0G1	THR	Α	87	28.486	38.558	41.887	1.00 20.57
ATOM	225	CG2	THR	Α	87	29.304	36.977	40.278	1.00 18.65
ATOM	226	N	LEU		88	26.972	34.907	39.701	1.00 18.38
•									
MOTA	227	CA	LEU		88	26.991	33.522	39.193	1.00 18.18
ATOM	228	C	LEU	Α	88	27.572	33.496	37.781	1.00 18.11
MOTA	229	0	LEU	Ά	88	27.353	34.457	36.974	1.00 18.86
ATOM	230	СВ			88				
			LEU			25.568	32.952	39.159	1.00 16.21
MOTA	231	CG	LEU		88	24.825	32.828	40.495	1.00 18.20
ATOM	232	CD1	LEU	A	88	23.366	32.474	40.226	1.00 18.10
ATOM	233		LEU		88	25.484	31.766	41.379	1.00 16.56
	234								
MOTA		N	ASN		89	28.317	32.443	37.459	1.00 15.84
MOTA	235	CA	ASN	A	89	28.876	32.312	36.101	1.00 16.22
ATOM	236	С	ASN	Α	89	27.841	31.544	35.300	1.00 16.03
ATOM	237	0	ASN		89	27.363	30.450	35.735	1.00 15.05
ATOM	238	CB	ASN		89	30.208	31.565	36.114	1.00 15.71
MOTA	239	CG	ASN		89	31.324	32.396	36.700	1.00 16.10
MOTA	240	OD1	ASN	Α	89	31.390	33.650	36.477	1.00 15.48
MOTA	241		ASN		89	32.217	31.750	37.439	1.00 14.07
ATOM	242	N							
			ILE		90	27.485	32.091	34.145	1.00 15.55
MOTA	243	CA	ILE		90	26.445	31.494	33.292	1.00 14.59
MOTA	244	С	ILE	Α	90	26.960	31.052	31.930	1.00 15.07

ATOM	245	0	ILE A	A 90	27.578	31.867	31.173	1.00 13.01
ATOM	246	СВ	ILE A			32.512		1.00 13.01
ATOM	247	CG1					33.084	-
						33.098	34.437	1.00 14.15
ATOM	248	CG2			24.114	31.847	32.407	1.00 14.29
MOTA	249	CD1			24.356	32.062	35.426	1.00 13.44
ATOM	250	N	LEU 2		26.714	29.790	31.590	1.00 15.08
ATOM	251	CA	LEU 2	A 91	27.153	29.249	30.284	1.00 15.63
MOTA	252	C	LEU 2	A 91	26.313	29.878	29.174	1.00 16.04
ATOM	253	0	LEU I	A 91	25.041	29.904	29.250	1.00 16.72
ATOM	254	СВ	LEU 2			27.721	30.265	1.00 14.67
ATOM	255	CG	LEU 2			26.945	29.012	1.00 15.49
ATOM	256		LEU I		27.692	25.485	29.364	
ATOM	257	CD2			26.393			1.00 15.10
	258					27.052	27.925	1.00 15.54
ATOM		N	VAL I		26.995	30.408	28.164	1.00 16.13
MOTA	259	CA	VAL I		26.336	31.051	27.003	1.00 15.39
MOTA	260	C	VAL 1		25.901	29.960	26.038	1.00 15.51
ATOM	261	О	VAL 2		26.761	29.243	25.440	1.00 16.92
MOTA	262	CB	VAL A	A 92	27.306	32.008	26.278	1.00 15.40
ATOM	263	CG1	VAL A	A 92	26.668	32.523	24.994	1.00 16.99
MOTA	264	CG2	VAL A	A 92	27.671	33.172	27.200	1.00 13.64
MOTA	265	N	ASP A		24.594	29.824	25.845	1.00 16.41
ATOM	266	CA	ASP A		24.069	28.762	24.974	1.00 14.41
ATOM	267	С	ASP Z		23.090	29.226	23.903	1.00 15.40
ATOM	268	ō ·	ASP A		21.889	29.494	24.206	
ATOM	269	СВ	ASP A		23.411			
ATOM	270	CG	ASP A			27.701	25.861	1.00 16.00
MOTA	271				22.897	26.512	25.078	1.00 16.45
			ASP A		23.536	26.133	24.076	1.00 17.23
ATOM	272		ASP A		21.863	25.938	25.481	1.00 16.68
MOTA	273	N	THR A		23.550	29.326	22.657	1.00 13.38
MOTA	274	CA	THR A		22.636	29.745	21.574	1.00 13.70
MOTA	275	С	THR A		21.811	28.549	21.109	1.00 13.68
ATOM	276	0	THR A	94	20.941	.28.671	20.190	1.00 14.18
MOTA	277	CB	THR A	94	23.397	30.349	20.362	1.00 14.99
MOTA	278	OG1	THR A	94	24.279	29.370	19.798	1.00 14.96
ATOM	279	CG2	THR A	94	24.201	31.568	20.794	1.00 14.04
MOTA	280	N	GLY A	<u>4</u> 95	22.053	27.392	21.719	1.00 14.90
MOTA	281	CA	GLY A		21.309	26.199	21.351	1.00 15.51
ATOM	282	С	GLY A	A 95	20.108	25.969	22.255	1.00 16.96
ATOM	283	Ō	GLY A		19.516	24.850	22.275	1.00 16.90
ATOM	284	N	SER A		19.721	26.987	23.011	1.00 10.30
ATOM	285	CA	SER A		18.562	26.851		
ATOM	286	C	SER A		17.990		23.922	1.00 17.95
ATOM	287	Ö				28.231	24.226	1.00 17.07
ATOM	288		SER A		18.573	29.269	23.803	1.00 14.94
ATOM		CB	SER A		19.005	26.174	25.219	1.00 18.55
	289	OG	SER A		19.640	26.894	26.276	1.00 26.99
ATOM	290	N	SER A		16.869	28.292	24.936	1.00 16.25
ATOM	291	CA	SER A		16.290	29.614	25.258	1.00 18.39
ATOM	292	C	SER A		15.740	29.776	26.670	1.00 17.83
ATOM	293	0	SER A		14.866	30.653	26.932	1.00 18.75
MOTA	294	CB	SER A	97	15.224	29.993	24.227	1.00 18.88
MOTA	295	OG	SER A	97	14.633	28.850	23.651	1.00 23.68
MOTA	296	N	ASN A	98	16.229	28.959	27.592	1.00 17.57
ATOM	297	CA	ASN A		15.809	29.073	28.993	1.00 16.01
MOTA	298	С	ASN A		16.963	29.611	29.821	1.00 16.51
ATOM	299	0	ASN A		18.127	29.109	29.709	1.00 16.69
ATOM	300	СВ	ASN A		15.401	27.720	29.566	1.00 13.74
ATOM	301	CG	ASN A		13.969	27.720	29.241	1.00 15.74
ATOM	302		ASN A		13.669	26.795	28.139	
ATOM	303		ASN A					1.00 13.27
ATOM	304	N	PHE A			27.680	30.158	1.00 13.26
ATOM	305	CA	PHE A		16.688	30.640	30.614	1.00 14.45
ATOM	306	CY	PHE A		17.710	31.196	31.519	1.00 13.19
	200	·	- 1111 F	99	17.453	30.424	32.812	1.00 13.23

MOTA	307	0	PHE	Α	99	16	.319	30.466	33.384	1.00 11.00
ATOM	308	CB	PHE	A	99	17	.491	32.699	31.722	1.00 13.54
ATOM	309	CG	PHE	Α	99	18	.390	33.318	32.761	1.00 14.79
ATOM	310	CD1	PHE	Α	99	19	.741	32.978	32.836	1.00 15.02
ATOM	311	CD2			99		.889	34.258	33.657	1.00 16.17
ATOM	312	CE1	PHE		99		.576	33.564	33.784	1.00 14.99
ATOM	313	CE2	PHE				.718	34.852	34.610	1.00 16.36
ATOM	314	CZ	PHE		99		.064	34.503	34.674	1.00 14.33
ATOM	315	N			100		.457	29.691	33.274	1.00 11.83
ATOM	316	CA	ALA	Α	100	18	.298	28.889	34.497	1.00 12.34
MOTA	317	С	ALA	Α	100	19	.594	28.836	35.277	1.00 14.53
ATOM	318	0	ALA	Α	100	20	.722	28.896	34.684	1.00 15.19
ATOM	319	CB	ALA	Α	100	17	.849	27.486	34.138	1.00 13.09
ATOM	320	N	VAT.	Α	101		.467	28.727	36.595	1.00 13.51
ATOM	321	CA	VAL				.640	28.686	37.473	1.00 13.80
ATOM	322	C			101		.429	27.693	38.610	1.00 15.86
	323		VAL							
ATOM		0					.253	27.424	39.031	1.00 13.90
ATOM	324	CB			101		.912	30.082	38.075	1.00 14.68
MOTA	325		VAL				.126	31.098	36.962	1.00 12.49
MOTA	326	CG2	VAL			19	.743	30.509	38.953	1.00 13.11
MOTA	327	N	GLY	Α	102	21	.528	27.120	39.098	1.00 16.51
ATOM	328	CA	GLY	A	102	21	.437	26.189	40.207	1.00 17.46
ATOM	329	С	GLY	Α	102	20	.858	26.966	41.375	1.00 19.61
MOTA	330	0	GLY	Α	102		.303	28.128	41.641	1.00 19.12
ATOM	331	N	ALA				.875	26.395	42.065	1.00 19.81
ATOM	332	CA	ALA				.241	27.092	43.212	1.00 22.41
ATOM	333	C	ALA				.098	26.169	44.414	1.00 22.41
			ALA							
ATOM	334	0					.196	26.366	45.293	1.00 24.50
ATOM	335	CB	ALA				.880	27.627	42.807	1.00 21.12
MOTA	336	N	ALA				.967	25.168	44.470	1.00 23.53
ATOM	337	ÇA	ALA				.979	24.180	45.566	1.00 24.47
ATOM	338	С	ALA				.341	23.505	45.517	1.00 24.98
ATOM	339	0	ALA	Α	104	21	.974	23.413	44.419	1.00 26.65
ATOM	340	CB	ALA	Α	104	18	.869	23.150	45.367	1.00 23.55
MOTA	341	N	PRO	Α	105	21	.836	23.026	46.668	1.00 25.27
ATOM	342	CA	PRO	Α	105		.140	22.361	46.733	1.00 24.87
ATOM	343	С	PRO	Α	105	23	.328	21.286	45.672	1.00 24.16
MOTA	344	0	PRO	Α	105	22	.350	20.594	45.251	1.00 24.35
ATOM	345	CB	PRO	Α	105	23	.159	21.778	48.143	1.00 25.36
MOTA	346	CG	PRO	Α	105	22	.347	22.763	48.920	1.00 25.71
MOTA	347	ĆD	PRO	Α	105	21	.183	23.020	47.990	1.00 25.99
ATOM	348	N	HIS	Α	106	24	.566	21.135	45.227	1.00 24.93
MOTA	349	CA	HIS				.918	20.119	44.223	1.00 23.63
ATOM	350	С	HIS				.402	19.843	44.367	1.00 24.29
ATOM	351	0	HIS				.207	20.790	44.596	1.00 24.19
ATOM	352	СВ	HIS				.646	20.622	42.807	1.00 24.15
ATOM	353	CG	HIS				.887	19.587	41.756	1.00 24.43
ATOM	354		HIS				.912	18.702	41.348	1.00 25.53
MOTA	355		HIS				.012	19.244	41.084	1.00 23.79
ATOM	356		HIS				.426		40.471	1.00 25.66
ATOM	357		HIS				.699	17.857		
ATOM	358	NEZ	PRO					18.164	40.294	1.00 24.92
							.811	18.572	44.236	1.00 25.36
ATOM	359	CA	PRO				.224	18.200	44.358	1.00 26.23
MOTA	360	С	PRO				.164	19.025	43.474	1.00 26.26
MOTA	361	0	PRO				.335	19.296	43.866	1.00 28.01
MOTA	362	CB	PRO	Α	107		.225	16.722	43.972	1.00 26.21
MOTA	363	CG	PRO			26	.875	16.259	44.418.	1.00 26.75
MOTA	364	CD	PRO	Α	107	25	.977	17.384	43.971	1.00 25.04
ATOM	365	N	PHE			28	. 695	19.435	42.299	1.00 25.94
ATOM	366	CA	PHE				.556	20.218	41.384	1.00 26.76
MOTA	367	С	PHE				.358	21.726	41.450	1.00 26.66
MOTA	368	0	PHE				.103	22.494	40.778	1.00 26.81
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ATOM	369	CB	PHE A	108	29.368	19.754	39.936	1.00 26.67
ATOM	370	CG	PHE A	108	29.665	18.300	39.720	1.00 26.80
ATOM	371		PHE A		30.531	17.614	40.569	1.00 27.67
MOTA	372		PHE A		29.090	17.615	38.655	1.00 27.12
MOTA	373		PHE A		30.819	16.262	40.359	1.00 27.99
MOTA	374	CE2	PHE A	108	29.369	16.267	38.433	1.00 26.65
ATOM	375	CZ	PHE A	108	30.235	15.587	39.286	1.00 26.94
MOTA	376	N	LEU A	109	28.386	22.180	42.231	1.00 26.14
ATOM	377	CA	LEU A		28.144	23.629	42.346	1.00 27.17
ATOM	378	C	LEU A		28.914	24.248	43.510	1.00 29.20
ATOM	379	o	LEU A		28.861	23.743	44.669	1.00 26.91
MOTA	380	CB	LEU A		26.647	23.911	42.498	1.00 25.73
ATOM	381	CG	LEU A		25.811	23.714	41.230	1.00 25.94
ATOM	382		LEU A		24.343	23.983	41.530	1,00 24.99
ATOM	383	CD2	LEU A	109	26.310	24.657	40.136	1.00 24.26
ATOM	384	N	HIS A	110	29.632	25.328	43.213	1.00 32.94
ATOM	385	CA	HIS A	110	30.442	26.077	44.207	1.00 35.82
MOTA	386	С	HIS A	110	29.533	27.015	44.983	1.00 33.93
ATOM	387	Ō	HIS A		29.732	27.265	46.209	1.00 34.20
ATOM	388	CB	HIS A		31.501	26.915	43.485	1.00 42.49
ATOM	389	CG	HIS A		32.907	26.469	43.732	1.00 47.84
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ATOM	390		HIS A		33.509	26.558	44.969	1.00 50.74
ATOM	391		HIS A		33.834	25.934	42.899	1.00 49.74
ATOM	392		HIS A		34.746	26.098	44.888	1.00 51.83
MOTA	393	NE2	HIS A	110	34.968	25.713	43.644	1.00 51.38
ATOM	394	N	ARG A	111	28.547	27.553	44.279	1.00 31.13
MOTA	395	CA	ARG A	111	27.579	28.494	44.857	1.00 28.72
ATOM	396	С	ARG A		26.287	28.331	44.072	1.00 28.16
ATOM	397	0	ARG A		26.267	27.652	43.000	1.00 27.40
ATOM	398	СВ	ARG A		28.108	29.924	44.717	1.00 28.09
ATOM	399	CG	ARG A		28.550	30.255	43.305	1.00 26.48
ATOM	400	CD	ARG A		29.216	31.616	43.201	1.00 25.86
ATOM	401	NE	ARG A		29.723	31.831	41.849	1.00 25.21
MOTA	402	CZ	ARG A		30.423	32.892	41.465	1.00 24.44
MOTA	403	NH1	ARG A	111	30.708	33.850	42.337	1.00 25.08
ATOM	404	NH2	ARG A	111	30.828	32.995	40.205	1.00 22.62
MOTA	405	N	TYR A	112	25.207	28.922	44.566	1.00 26.27
MOTA	406	CA	TYR A	112	23.922	28.814	43.866	1.00 23.70
ATOM	407	С	TYR A	112	22.955	29.916	44.250	1.00 22.77
ATOM	408	Ó	TYR A		23.140	30.633	45.283	1.00 21.10
ATOM	409	СВ	TYR A		23.295	27.437	44.119	1.00 25.47
ATOM	410	CG	TYR A		23.036	27.111	45.575	1.00 27.20
ATOM	411		TYR A		21.885		-	1.00 27.20
ATOM	412		TYR A		23.946	27.569 26.353	46.222 46.309	1.00 27.51
MOTA	413		TYR A		21.647	27.276	47.565	1.00 27.78
MOTA	414	CE2			23.720	26.058	47.651	1.00 28.63
MOTA	415	CZ	TYR A		22.570	26.522	48.270	1.00 28.98
MOTA	416	OH	TYR A		22.352	26.228	49.591	1.00 30.28
MOTA	417	N	TYR A	113	21.927	30.069	43.428	1.00 19.32
MOTA	418	CA	TYR A	113	20.896	31.090	43.624	1.00 18.94
MOTA	419	С	TYR A	113	20.047	30.807	44.857	1.00 17.90
MOTA	420	, O	TYR A	113	19.480	29.688	45.011	1.00 19.37
MOTA	421	СВ	TYR A		20.027	31.141	42.369	1.00 17.76
MOTA	422	CG	TYR A		18.887	32.135	42.378	1.00 17.68
MOTA	423		TYR A		19.024	33.397	42.963	1.00 16.86
ATOM	424		TYR A					1.00 16.79
					17.709	31.854	41.688	
MOTA	425		TYR A		18.020	34.349	42.848	1.00 17.05
MOTA	426				16.704	32.796	41.563	1.00 16.02
MOTA	427	CZ	TYR A		16.858	34.038	42.138	1.00 17.36
MOTA	428	OH	TYR A		15.848	34.963	41.984	1.00 16.62
ATOM	429	N	GLN A		19.967	31.790	45.746	1.00 18.68
MOTA	430	CA	GLN A	114	19.156	31.673	46.983	1.00 20.28

ATOM	431	С	GLN A		18.057	32.719	46.897	1.00 19.59
MOTA	432	0	GLN A		18.285	33.933	47.192	1.00 20.34
MOTA	433	CB	GLN A	114	20.028	31.912	48.216	1.00 19.79
ATOM	434	CG	GLN A	114	21.048	30.814	48.434	1.00 22.79
ATOM	435	CD	GLN A		21.942	31.063	49.626	1.00 24.34
ATOM	436	OE1						
					22.708	32.073	49.668	1.00 26.47
MOTA	437	NE2			21.876	30.173	50.606	1.00 24.49
MOTA	438	N	ARG A		16.876	32.275	46.479	1.00 20.48
MOTA	439	CA	ARG A	115	15.703	33.159	46.305	1.00 21.24
MOTA	440	С	ARG A	115	15.234	33.837	47.583	1.00 21.94
MOTA	441	0	ARG A	115	14.784	35.022	47.546	1.00 21.40
ATOM	442	СВ	ARG A		14.550	32.366	45.686	1.00 20.21
ATOM	443	CG	ARG A		14.807	31.953	44.240	1.00 20.21
ATOM	444	CD	ARG A					
					13.917	30.796	43.824	1.00 20.32
ATOM	445	NE	ARG A		14.305	29.567	44.508	1.00 20.45
MOTA	446	CZ	ARG A		13.626	28.428	44.448	1.00 19.47
MOTA	447	NH1	ARG A		12.514	28.352	43.732	1.00 20.02
ATOM	448	NH2	ARG A	115	14.061	27.366	45.106	1.00 21.63
ATOM	449	N	GLN A	116	15.323	33.138	48.710	1.00 22.93
MOTA	450	CA	GLN A	116	14.880	33.723	49.993	1.00 24.99
ATOM	451	C	GLN A		15.718	34.953	50.343	1.00 23.86
ATOM	452	ō	GLN A		15.242			
						35.873	51.080	1.00 24.27
MOTA	453	CB	GLN A		14.972	32.691	51.123	1.00 27.81
ATOM	454	CG	GLN A		16.391	32.280	51.502	1.00 32.89
ATOM	455	CD	GLN A		16.999	31.257	50.550	1.00 36.05
ATOM	456	OE1	GLN A	116	16.955	31.423	49.295	1.00 36.88
ATOM	457	NE2	GLN A	116	17.577	30.199	51.112	1.00 37.21
MOTA	458	N	LEU A	117	16.944	35.006	49.833	1.00 20.91
MOTA	459	CA	LEU A	117	17.831	36.153	50.112	1.00 20.59
ATOM	460	C	LEU A		17.673	37.296	49.124	1.00 20.35
ATOM	461	o	LEU A		18.440			
						38.301	49.191	1.00 18.93
ATOM	462	CB	LEU A		19.296	35.707	50.128	1.00 21.68
ATOM	463	CG	LEU A		19.887	35.224	51.454	1.00 22.49
MOTA	464		LEU A		19.001	34.175	52.074	1.00 22.63
MOTA	465	CD2	LEU A	117	21.286	34.675	51.210	1.00 22.12
MOTA	466	N	SER A	118	16.714	37.183	48.210	1.00 18.14
MOTA	467	CA	SER A	118	16.484	38.252	47.208	1.00 17.08
ATOM	468	С	SER A		15.150	38.953	47.436	1.00 16.25
MOTA	469	0	SER A		14.055	38.316	47.347	1.00 16.00
ATOM	470	СB	SER A		16.519	37.679	45.787	1.00 15.12
ATOM	471	OG	SER A		16.301			
ATOM	472		SER A			38.708	44.835	1.00 16.81
		N			15.210	40.250	47.711	1.00 15.31
ATOM	473	CA	SER A		13.991	41.044	47.973	1.00 18.09
MOTA	474	С	SER A		13.169	41.307	46.714	1.00 17.35
MOTA	475	0	SER A		11.964	41.669	46.800	1.00 17.62
MOTA	476	CB	SER A	119	14.371	42.380	48.618	1.00 16.85
ATOM	477	OG	SER A	119	15.158	43.160	47.727	1.00 18.71
ATOM	478	N	THR A		13.781	41.137	45.546	1.00 18.90
ATOM	479	CA	THR A		13.075	41.381	44.263	1.00 17.26
ATOM	480	C	THR A		12.587			
ATOM	481	0				40.104	43.594	1.00 17.17
			THR A		12.004	40.139	42.466	1.00 18.70
ATOM	482	CB	THR A		13.980	42.143	43.283	1.00 17.78
MOTA	483		THR A		15.305	41.609	43.355	1.00 17.35
MOTA	484	CG2	THR A	120	14.012	43.630	43.624	1.00 17.37
MOTA	485	N	TYR A	121	12.800	38.977	44.257	1.00 18.03
MOTA	486	CA	TYR A	121	12.364	37.676	43.715	1.00 18.53
MOTA	487	C	TYR A		10.841	37.584	43.606	1.00 18.12
MOTA	488	ō	TYR A		10.088	38.028	44.531	1.00 19.29
ATOM	489	СВ	TYR A		12.878			
ATOM	490	CG				36.547	44.607	1.00 18.32
			TYR A		12.187	35.225	44.368	1.00 22.03
ATOM	491		TYR A		12.429	34.484	43.209	1.00 21.48
ATOM	492	CDZ	TYR A	171	11.268	34.725	45.291	1.00 21.95

ATOM	493	CE1	TYR A	121	11.776	33.280	42.977	1.00 21.33
MOTA	494	CE2	TYR A	121	10.608	33.523	45.067	1.00 22.77
ATOM	495	CZ	TYR A	121	10.867	32.807	43.908	1.00 23.35
MOTA	496	OH	TYR A		10.206	31.622	43.682	1.00 23.63
MOTA	497	N	ARG A		10.365	37.039	42.492	1.00 16.86
MOTA	498	CA	ARG A		8.909	36.851	42.281	1.00 16.79
ATOM	499	C	ARG A	122	8.703	35.397	41.890	1.00 17.46
ATOM	500	0	ARG A	122	9.348	34.884	40.924	1.00 17.88
ATOM	501	СВ	ARG A		8.384	37.764	41.174	1.00 14.87
MOTA	502	CG	ARG A		8.335	39.230	41.548	
MOTA	503	CD	ARG A		7.895	40.067	40.369	1.00 14.98
ATOM	504	NE	ARG A	122	7.822	41.481	40.706	1.00 16.19
ATOM	505	CZ	ARG A	122	7.546	42.442	39.833	1.00 16.67
MOTA	506	NH1	ARG A	122	7.316	42.142	38.559	1.00 15.67
ATOM	507	NH2	ARG A	122	7.505	43.704	40.233	1.00 16.38
ATOM	508	N	ASP A		7.836	34.720	42.628	1.00 18.52
MOTA	509	CA	ASP A		7.538	33.296	42.388	1.00 19.00
MOTA	510	C	ASP A		6.435	33.147	41.347	1.00 19.87
ATOM	511	0	ASP A		5.342	33.757	41.490	1.00 17.59
MOTA	512	CB	ASP A	123	7.090	32.657	43.702	1.00 19.80
ATOM	513	CG	ASP A		6.841	31.171	43.582	1.00 20.76
ATOM	514		ASP A		6.933	30.615	42.463	1.00 20.41
ATOM	515		ASP A		6.549	30.559	44.629	1.00 22.50
MOTA	516	N	LEU A		6.689	32.359	40.305	1.00 20.70
ATOM	517	CA	LEU A		5.672	32.139	39.255	1.00 21.20
MOTA	518	С	LEU A	124	4.790	30.929	39.562	1.00 21.64
MOTA	519	0	LEU A	124	3.832	30.601	38.786	1.00 21.17
ATOM	520	CB	LEU A	124	6.343	31.978	37.888	1.00 21.51
ATOM	521	CG	LEU A		6.850	33.288	37.270	1.00 22.05
ATOM	522		LEU A		7.617	32.994	35.997	1.00 22.03
ATOM	523	CD2	LEU A		5.678	34.217	36.983	1.00 21.49
ATOM	524	N	ARG A		5.083	30.252	40.666	1.00 22.67
ATOM	525	CA	ARG A	125	4.286	29.078	41.085	1.00 25.58
MOTA	526	С	ARG A	125	4.106	28.081	39.944	1.00 26.39
MOTA	527	0	ARG A	125	2.974	27.552	39.719	1.00 26.83
MOTA	528	СВ	ARG A		2.918	29.553	41.593	1.00 26.62
ATOM	529	CG	ARG A		3.016	30.511	42.783	1.00 30.02
ATOM	530	CD	ARG A		1.733	31.311	43.002	1.00 30.02
ATOM	531	NE	ARG A		1.910	32.334	44.034	1.00 36.63
MOTA	532	CZ	ARG A		1.049	33.323	44.282	1.00 38.12
MOTA	533	NH1	ARG A	125	-0.070	33.441	43.575	1.00 37.55
MOTA	534	NH2	ARG A	125	1.307	34.202	45.240	1.00 38.11
MOTA	535	N	LYS A	126	5189	27.810	39.221	1.00 26.62
MOTA	536	CA	LYS A		5.162	26.861	38.079	1.00 26.41
ATOM	537	C	LYS A		6.453	26.063	37.986	1.00 24.61
ATOM	538							
		0	LYS A		7.577	26.624	38.141	1.00 22.46
MOTA	539	CB	LYS A		4.971	27.605	36.756	1.00 28.55
MOTA	540	CG	LYS A		3.539	27.804	36.326	1.00 32.76
ATOM	541	CD	LYS A	126	3.486	28.380	34.917	1.00 36.53
ATOM	542	CE	LYS A	126	2.048	28.607	34.456	1.00 38.52
ATOM	543	NZ	LYS A	126	1.234	27.355	34.550	1.00 40.78
ATOM	544	N	GLY A		6.326	24.770	37.731	1.00 23.25
ATOM	545	CA	GLY A					
					7.504	23.941	37.598	1.00 22.82
MOTA	546	C	GLY A		7.970	23.995	36.157	1.00 22.77
MOTA	547	0	GLY A		7.220	24.487	35.252	1.00 22.00
ATOM	548	N	VAL A		9.184	23.521	35.909	1.00 21.58
MOTA	549	CA	VAL A	128	9.731	23.511	34.541	1.00 22.39
MOTA	550	С	VAL A	128	10.736	22.388	34.390	1.00 21.31
ATOM -	551	0	VAL A		11.547	22.101	35.323	1.00 21.59
ATOM	552	СВ	VAL A		10.416	24.851	34.180	1.00 21.77
ATOM	553		VAL A		11.572		35.122	1.00 22.15
						25.120		
MOTA	554	CGZ	VAL A	120	10.903	24.809	32.740	1.00 23.66

ATOM	555	N	TYR	A	129	10.700	21.744	33.233	1.00 21.64
ATOM	556	CA	TYR	Α	129	11.598	20.624	32.933	1.00 21.55
MOTA	557	С	TYR	Α	129	12.298	20.882	31.609	1.00 20.25
ATOM	558	0	TYR			11.635	21.188	30.573	1.00 20.01
MOTA	559	CB	TYR			10.785	19.333	32.841	1.00 23.37
MOTA	560	CG	TYR			11.545	18.164	32.271	1.00 26.64
MOTA	561	CD1	TYR	Α	129	12.628	17.613	32.956	1.00 27.70
MOTA	562	CD2	TYR	Α	129	11.178	17.598	31.048	1.00 27.27
MOTA	563		TYR			13.323	16.529	32.443	1.00 29.33
MOTA	564		TYR			11.872	16.507	30.524	1.00 28.75
MOTA	565	CZ	TYR			12.942	15.980	31.231	1.00 28.91
ATOM	566	OH	TYR	A	129	13.634	14.896	30.751	1.00 30.21
ATOM	567	N	VAL	Α	130	13.620	20.782	31.602	1.00 19.35
ATOM	568	CA	VAL			14.353	21.003	30.350	1.00 17.21
ATOM	569	C	VAL			15.308	19.872	30.022	1.00 16.02
ATOM	570	0	VAL			16.319	19.628	30.748	1.00 16.89
ATOM	571	CB	VAL	Α	130	15.136	22.334	30.370	1.00 17.86
ATOM	572	CG1	VAL	Α	130	15.934	22.485	29.075	1.00 15.31
ATOM	573	CG2	VAL	Α	130	14.163	23.505	30.525	1.00 15.67
ATOM	574	N .	PRO			15.013	19.136	28.945	1.00 14.83
ATOM	575	CA	PRO			15.868	18.028	28.529	1.00 14.77
MOTA	576	С	PRO			16.743	18.516	27.372	1.00 15.00
MOTA	577	0	PRO	Α	131	16.234	19.154	26.402	1.00 15.43
ATOM	578	CB	PRO	Α	131	14.857	16.971	28.106	1.00 13.57
ATOM	579	CG	PRO	Α	131	13.809	17.806	27.421	1.00 13.44
ATOM	580	CD				13.706	19.078	28.262	1.00 13.99
			PRO						
MOTA	581	N	TYR			18.043	18.268	27.465	1.00 14.75
ATOM	582	CA	TYR	Α	132	18.989	18.679	26.404	1.00 17.37
MOTA	583	С	TYR	Α	132	19.438	17.415	25.676	1.00 17.52
ATOM	584	0	TYR	Α	132	19.100	16.274	26.105	1.00 17.41
ATOM	585	СB	TYR			20.211	19.369	27.020	1.00 16.93
MOTA	586	CG	TYR			19.909	20.665	27.742	1.00 18.63
ATOM	587	CD1	TYR	A	132	19.834	21.881	27.051	1.00 17.88
MOTA	588	CD2	TYR	Α	132	19.706	20.681	29.122	1.00 19.01
ATOM	589	CE1	TYR	Α	132	19.564	23.080	27.722	1.00 16.57
ATOM	590		TYR			19.435	21.867	29.799	1.00 17.74
ATOM	591	CZ	TYR			19.365	23.062	29.098	1.00 19.02
MOTA	592	OH	TYR			19.083	24.229	29.782	1.00 18.23
MOTA	593	N	THR			20.188	17.574	24.592	1.00 18.46
ATOM	594	CA	THR	Α	133	20.686	16.403	23.842	1.00 18.54
MOTA	595	С	THR	Α	133	21.525	15.580	24.812	1.00 20.42
ATOM	596	0	THR	Α	133	21.667	14.325	24.672	1.00 19.49
AŤOM	597	СВ	THR			21.546	16.846	22.653	1.00 18.40
			THR			20.720	17.539	21.708	1.00 20.46
ATOM	598								
MOTA	599		THR			22.194	15.645	21.976	1.00 18.37
MOTA	600	N	GLN	A	134	22.064	16.265	25.810	1.00 22.23
MOTA	601	CA	GLN	Α	134	22.890	15.624	26.842	1.00 24.27
MOTA	602	С	GLN	Α	134	22.723	16.406	28.140	1.00 23.32
MOTA	603	ō	GLN			23.179	17.580	28.252	1.00 21.03
MOTA	604	CB	GLN			24.352	15.633	26.405	1.00 28.22
MOTA	605	CG	GLN			25.140	14.412	26.808	1.00 32.76
MOTA	606	CD	GLN	Α	134	25.020	13.296	25.781	1.00 36.63
ATOM	607	OE1	GLN	Α	134	26.052	12.680	25.356	1.00 37.34
MOTA	608		GLN			23.791	13.018	25.352	1.00 38.92
ATOM	609	N	GLY			22.080	15.789	29.124	1.00 23.28
ATOM	610	CA	GLY			21.863	16.460	30.391	1.00 21.50
MOTA	611	С	GLY			20.432	16.946	30.483	1.00 22.11
MOTA	612	0	GLY	Α	135	19.735	17.111	29.435	1.00 20.68
MOTA	613	N	LYS	Α	136	19.968	17.190	31.703	1.00 22.97
MOTA	614	CA	LYS			18.584	17.654	31.923	1.00 23.80
ATOM	615	C	LYS			18.429		33.353	1.00 22.33
							18.147		
MOTA	616	0	LYS	H	730	19.196	17.719	34.269	1.00 21.42

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MOTA	617	CB	LYS	A	136	17.606	16.501	31.677	1.00 25.37
MOTA	618	CG	LYS			17.823	15.310	32.607	1.00 28.29
MOTA	619	CD	LYS	Α	136	16.804	14.196	32.374	1.00 31.54
ATOM	620	CE	LYS			16.955	13.570	31.000	1.00 34.21
ATOM	621	NZ	LYS			15.996	12.444	30.789	1.00 37.76
MOTA	622	N	TRP			17.470	19.040	33.573	1.00 21.02
ATOM	623	CA	TRP			17.214	19.562	34.928	1.00 20.75
MOTA	624	C	TRP	Α	137	15.750	19.907	35.133	1.00 20.62
MOTA	625	0	TRP	A	137	14.951	19.978	34.153	1.00 20.05
MOTA	626	CB	TRP	Α	137	18.077	20.800	35.231	1.00 18.46
ATOM	627	CG	TRP	Α	137	17.960	21.937	34.248	1.00 18.02
MOTA	628	CD1	TRP	Α	137	18.865	22.276	33.281	1.00 18.12
MOTA	629	CD2				16.881	22.879	34.134	1.00 17.27
MOTA	630		TRP			18.419	23.369	32.574	1.00 17.78
ATOM	631	CE2				17.204	23.758	33.074	1.00 17.40
ATOM	632	CE3	TRP	Α	137	15.675	23.067	34.823	1.00 17.08
ATOM	633	CZ2	TRP			16.363	24.807	32.684	1.00 15.50
MOTA	634	CZ3	TRP			14.836	24.113	34.434	1.00 17.23
ATOM	635	CH2				15.188	24.968	33.373	1.00 17.46
ATOM	636	N	GLU			15.385	20.098	36.395	1.00 21.53
MOTA	637	CA	GLU			14.014	20.472	36.789	1.00 24.94
MOTA	638	С	GLU			14.166	21.642	37.745	1.00 23.18
MOTA	639	0	GLU			15.168	21.719	38.526	1.00 21.21
ATOM	640	CB	GLU			13.320	19.320	37.515	1.00 28.46
ATOM	641	CG	GLU			13.053	18.101	36.656	1.00 34.91
ATOM	642	CD	GLU			12.562	16.919	37.472	1.00 37.93
ATOM	643		GLU			12.175	15.897	36.864	1.00 40.28
ATOM	644	OE2				12.570	17.009	38.722	1.00 40.20
ATOM	645	N	GLY			13.214	22.559	37.711	1.00 22.13
ATOM	646	CA	GLY			13.298	23.693	38.604	1.00 22.60
ATOM	647	C	GLY			11.975	24.402	38.713	1.00 21.54
ATOM	648	0	GLY			10.949	23.953	38.116	1.00 23.29
ATOM	649	N			140	11.962	25.494	39.465	1.00 21.74
ATOM	650	CA	GLU			10.733	26.284	39.648	1.00 21.81
ATOM	651	C	GLU			10.900	27.646	38.998	1.00 19.04
ATOM	652 653	0			140 .	11.975	28.304	39.125	1.00 18.42
ATOM ATOM	654	CB CG	GLU GLU			10.404 11.479	26.425 25.887	41.139 42.065	1.00 24.39
ATOM	655	CD	GLU			10.922	25.385	42.065	1.00 28.61
ATOM	656	OE1				10.322	24.297	43.389	1.00 29.72 1.00 31.43
ATOM	657	OE2	GLU			11.091	26.077	44.410	1.00 31.43
ATOM	658	N	LEU			9.870	28.071	38.278	1.00 30.48
ATOM	659	CA	LEU			9.901	29.360	37.585	1.00 15.48
ATOM	660	C	LEU			9.674	30.546	38.511	1.00 15.68
ATOM	661	Ō			141	8.832	30.499	39.466	1.00 13.45
ATOM	662		LEU			8.864	29.376	36.460	1.00 15.23
ATOM	663	CG			141	9.145	28.412	35.300	1.00 16.27
MOTA	664		LEU			8.008	28.461	34.300	1.00 15.60
ATOM	665		LEU			10.458	28.785	34.627	1.00 16.48
ATOM	666	N			142	10.424	31.608	38.241	1.00 15.15
MOTA	667	CA			142	10.323	32.819	39.015	1.00 12.33
ATOM	668	С	GLY	Α	142	10.845	33.953	38.167	1.00 14.67
MOTA	669	0	GLY	A	142	11.242	33.758	36.971	1.00 13.75
ATOM	670	N	THR	A	143	10.877	35.137	38.754	1.00 14.88
ATOM	671	CA	THR	A	143	11.354	36.324	38.050	1.00 15.26
MOTA	672	C	THR	A	143	12.262	37.103	39.008	1.00 14.53
MOTA	673	0			143	12.119	36.991	40.269	1.00 13.46
ATOM	674	СВ	THR			10.131	37.154	37.600	1.00 16.18
ATOM	675	OG1				10.192	37.362	36.187	1.00 20.69
ATOM	676	CG2				10.058	38.465	38.325	1.00 12.43
ATOM	677	N			144	13.202	37.866	38.466	1.00 14.22
ATOM	678	CA	ASP	A	144	14.117	38.652	39.321	1.00 15.38

ATOM	679	С	ASP			14.942	39.609	38.479	1.00 15.67
MOTA	680	0	ASP	Α	144	14.984	39.496	37.208	1.00 16.83
ATOM	681	CB	ASP	Α	144	15.063	37.721	40.086	1.00 15.20
MOTA	682	CG	ASP	Α	144	15.367	38.218	41.496	1.00 17.84
ATOM	683		ASP			15.359	39.447	41.724	1.00 16.62
ATOM	684		ASP			15.630	37.373	42.379	1.00 16.33
			LEU			15.596		39.147	1.00 16.74
ATOM	685	N					40.551		
ATOM	686	CA	LEU			16.442	41.537	38.454	1.00 18.66
ATOM	687	C	LEU	Α	145	17.757	40.854	38.101	1.00 20.21
ATOM	688	0	LEU	Α	145	18.381	40.147	38.961	1.00 21.75
ATOM	689	CB	LEU	A	145	16.697	42.746	39.351	1.00 18.43
MOTA	690	CG	LEU	Α	145	15.452	43.522	39.786	1.00 19.69
ATOM	691	CD1	LEU	Α	145	15.878	44.720	40.628	1.00 19.11
ATOM	692		LEU			14.660	43.971	38.557	1.00 18.50
ATOM	693	N	VAL			18.186	41.030	36.858	1.00 20.48
ATOM	694	CA	VAL			19.426	40.402	36.387	1.00 21.21
			VAL						1.00 21.21
ATOM	695	C				20.331	41.426	35.725	
ATOM	696	0	VAL			19.849	42.386	35.045	1.00 22.16
MOTA	697	CB	VAL			19.118	39.265	35.373	1.00 20.39
ATOM	698		VAL			20.405	38.575	34.941	1.00 20.39
ATOM	699	CG2	VAL	Α	146	18.163	38.261	35.998	1.00 17.90
ATOM	700	N	SER	Α	147	21.633	41.251	35.913	1.00 22.35
ATOM	701	CA	SER	Α	147	22.615	42.158	35.309	1.00 23.39
ATOM	702	C	SER	Α	147	23.829	41.383	34.833	1.00 21.77
ATOM	703	0	SER			24.119	40.242	35.321	1.00 20.08
ATOM	704	СВ	SER			23.059	43.225	36.316	1.00 25.41
ATOM	705	OG	SER			21.993	44.107	36.627	1.00 31.97
	706				148	24.534		33.878	1.00 19.69
ATOM		N					41.972		
ATOM	707	CA	ILE			25.757	41.377	33.329	1.00 19.14
ATOM	708	C			148	26.853	42.405	33.614	1.00 18.85
ATOM	709	0			148	27.021	43.408	32.853	1.00 17.87
ATOM	710	CB			148	25.618	41.137	31.817	1.00 18.61
ATOM	711	CG1	ILE			24.449	40.181	31.559	1.00 19.01
ATOM	712	CG2				26.909	40.564	31.255	1.00 17.68
MOTA	713	CD1	ILE	Α	148	24.221	39.864	30.097	1.00 19.61
MOTA	714	N	PRO	Α	149	27.601	42.214	34.711	1.00 17.99
ATOM	715	CA	PRO	Α	149	28.679	43.134	35.095	1.00 21.17
ATOM	716	С	PRO	Α	149	29.523	43.638	33.926	1.00 22.18
ATOM	717	0	PRO	Α	149	29.800	44.869	33.823	1.00 24.08
ATOM	718	CB	PRO	Α	149	29.485	42.317	36.103	1.00 19.87
ATOM	719	CG			149	28.404	41.529	36.797	1.00 19.57
MOTA	720	CD	PRO			27.542	41.061	35.628	1.00 17.55
ATOM	721	N	HIS			29.930	42.733		1.00 23.43
ATOM	722	CA	HIS			30.748	43.119	31.869	1.00 23.84
ATOM	723	C	HIS			29.933	43.067	30.588	1.00 24.47
MOTA	724	ŏ	HIS			30.334	42.431	29.566	1.00 25.89
ATOM	725	СВ	HIS			31.968	42.211	31.765	1.00 23.54
ATOM	726	CG	HIS			32.880	42.313	32.945	1.00 26.15
MOTA	727		HIS			33.619	43.446	33.216	1.00 27.28
MOTA	728		HIS			33.149	41.439	33.943	1.00 26.32
MOTA	729		HIS			34.305	43.264	34.330	1.00 27.48
ATOM	730	NE2	HIS			34.038	42.055	34.791	1.00 28.01
MOTA	731	N			151	28.785	43.727	30.630	1.00 25.49
MOTA	732	CA	GLY			27.906	43.784	29.485	1.00 26.41
ATOM	733	С	GLY	Α	151	27.325	45.179	29.468	1.00 27.16
ATOM	734	0	GLY	Α	151	27.981	46.136	29.983	1.00 26.97
ATOM	735	N			152	26.125	45.370	28.903	1.00 28.12
ATOM	736	CA			152	25.540	46.712	28.880	1.00 28.75
ATOM	737	C			152	25.219	47.165	30.304	1.00 30.53
MOTA	738	ō	PRO			24.844	46.331	31.182	1.00 28.62
ATOM	739	СВ			152	24.294	46.528	28.017	1.00 29.49
ATOM	740	CG			152	23.897	45.105	28.303	1.00 29.85
						~~.~,	30.100	20.303	

MOTA	741	CD	PRO				25.227	44.385	28.277	1.00 28.15
ATOM	742	N	ASN	Α	153		25.375	48.457	30.560	1.00 33.03
ATOM	743	CA	ASN	A	153		25.111	49.016	31.902	1.00 34.39
MOTA	744	С	ASN	Α	153		23.604	49.096	32.144	1.00 33.81
ATOM	745	0	ASN				23.009	50.218	32.222	1.00 33.63
ATOM	746	СВ	ASN		_		25.755	50.401	32.009	1.00 37.16
ATOM	747	CG	ASN				25.680	50.978	33.406	1.00 38.88
ATOM	748		ASN				25.974			
								50.272	34.416	1.00 40.17
ATOM	749		ASN				25.309	52.251	33.504	1.00 39.91
MOTA	750	N	VAL				22.971	47.934	32.265	1.00 31.55
MOTA	751	CA	VAL				21.514	47.872	32.486	1.00 29.59
ATOM	752	С	VAL				21.113	46.739	33.418	1.00 29.47
MOTA	753	О	VAL				21.924	45.809	33.718	1.00 30.24
MOTA	754	CB	VAL				20.755	47.681	31.154	1.00 29.95
ATOM	755	CG1	VAL	A	154		20.990	48.875	30.242	1.00 29.70
MOTA	756	CG2	VAL	Α	154		21.216	46.397	30.474	1.00 28.94
ATOM	757	N	THR	Α	155		19.874	46.799	33.882	1.00 27.83
MOTA	758	CA	THR	Α	155		19.323	45.773	34.779	1.00 27.61
ATOM	759	С	THR	Α	155		17.918	45.472	34.296	1.00 26.01
ATOM	760	0	THR	Α	155		17.114	46.413	34.041	1.00 27.70
MOTA	761	СВ	THR	Α	155		19.268	46.280	36.229	1.00 27.24
ATOM	762	OG1	THR	Α	155		20.603	46.486	36.703	1.00 29.54
ATOM	763	CG2	THR				18.573	45.270	37.129	1.00 27.37
ATOM	764	N	VAL				17.592	44.197	34.143	1.00 24.69
ATOM	765	CA	VAL				16.241	43.847	33.672	1.00 24.32
ATOM	766	C	VAL				15.631	42.736	34.504	1.00 23.23
MOTA	767	0	VAL				16.364	41.920	35.154	1.00 23.23
ATOM .	768	Св	VAL				16.253	43.402	32.184	1.00 25.34
ATOM	769		VAL				17.178	44.302	31.379	1.00 25.54
ATOM	770		VAL				16.684	41.960	32.063	1.00 24.89
ATOM	771	N .			157	•	14.306	42.687	34.521	1.00 21.44
ATOM	772	CA	ARG			: •	13.613	41.626	35.262	1.00 20.90
ATOM	773	С			157	•	13.374	40.560	34.215	1.00 20.13
ATOM	774	0	ARG		•		12.746	40.836	33.152	1.00 19.99
ATOM	775	CB	ARG				12.280	42.121	35.830	1.00 20.03
ATOM	776	CG	ARG				11.528	41.053	36.621	1.00 18.95
ATOM	777	CD	ARG				10.271	41.616	37.260	1.00 18.99
MOTA	778	NE	ARG				10.554	42.408	38.456	1.00 18.47
MOTA	779	CZ			157		10.973	41.902	39.613	1.00 19.19
MOTA	780		ARG				11.167	40.596	39.747	1.00 18.30
ATOM	781	NH2	ARG	Α	157		11.178	42.703	40.650	1.00 15.82
MOTA	782	N	ALA	Α	158		13.878	39.359	34.463	1.00 20.27
ATOM	783	CA	ALA	Α	158		13.713	38.266	33.496	1.00 19.08
MOTA	784	С	ALA	Α	158		13.279	36.986	34.175	1.00 19.45
ATOM	785	0	ALA	Α	158		13.379	36.845	35.432	1.00 19.64
ATOM	786	CB	ALA	Α	158		15.017	38.031	32.756	1.00 18.56
ATOM	787	N	ASN	Α	159		12.792	36.053	33.370	1.00 18.08
ATOM	788	CA	ASN	Α	159		12.363	34.756	33.876	1.00 18.21
ATOM	789	С			159		13.607	33.992	34.282	1.00 18.60
ATOM	790	0			159		14.666	34.033	33.577	1.00 19.42
ATOM	791	CB			159		11.601	33.992	32.797	1.00 16.91
ATOM	792	CG			159		10.282	34.647	32.459	1.00 18.46
ATOM	793		ASN			-	9.479	34.978	33.381	1.00 19.46
ATOM	794		ASN				10.020	34.848	31.174	1.00 16.51
MOTA	795	N			160		13.518	33.311	35.412	1.00 18.73
ATOM	796	CA			160		14.643	32.529	35.916	1.00 17.64
ATOM	797	C			160		14.112	31.191	36.373	1.00 17.04
ATOM	798	0			160		13.122	31.125	37.176	1.00 19.09
ATOM	790 799	CB			160		15.122	33.212	37.176	1.00 18.36
MOTA	800		ILE				15.764	34.629	36.758	1.00 17.90
ATOM	801	CG2			160		16.521	32.394	37.585	1.00 17.16
MOTA	802	CDI	ILE	A	TOO		16.521	35.336	37.875	1.00 18.56

ATOM	803	N	ALA			14.717	30.123	35.871	1.00 17.55
ATOM	804	CA	ALA			14.314	28.778	36.275	1.00 18.11
ATOM	805	C	ALA	A	161	15.267	28.394	37.399	1.00 18.26
MOTA	806	Ο.	ALA	A	161	16.507	28.223	37.166	1.00 17.61
MOTA	807	CB	ALA	Α	161	14.447	27.805	35.105	1.00 17.28
MOTA	808	N	ALA	Α	162	14.737	28.283	38.614	1.00 17.99
MOTA	809	CA	ALA	Α	162	15.567	27.901	39.775	1.00 18.02
ATOM	810	С	ALA	Α	162	15.746	26.382	39.774	1.00 18.52
ATOM	811	0	ALA	Α	162	14.835	25.619	40.207	1.00 18.43
ATOM	812	CB	ALA			14.897	28.359	41.067	1.00 17.36
ATOM	813	N	ILE			16.900	25.928	39.300	1.00 17.30
ATOM	814	CA	ILE			17.204	24.480	39.215	1.00 19.89
ATOM	815	C	ILE			17.314	23.802	40.577	1.00 20.34
ATOM	816	Õ	ILE			18.238	24.122	41.402	1.00 20.34
ATOM	817	СВ	ILE			18.512	24.245	38.430	
ATOM	818	CG1				18.347	24.753		1.00 17.19
ATOM	819	CG2	ILE			18.874	24.753	36.994	1.00 16.02
ATOM	820	CD1	ILE			19.628		38.445	1.00 14.93
ATOM	821	N	THR				24.735	36.174	1.00 16.24
ATOM	822	CA				16.409	22.860	40.826	1.00 20.42
ATOM	823		THR			16.379	22.122	42.112	1.00 23.01
		C	THR .			16.817	20.665	41.958	1.00 24.30
ATOM	824	0	THR .			17.119	19.966	42.973	1.00 26.25
ATOM	825	CB	THR .			14.966	22.173	42.735	1.00 22.01
ATOM	826	OG1				13.990	21.799	41.754	1.00 22.15
MOTA	827	CG2	THR .			14.656	23.584	43.214	1.00 22.73
ATOM	828	N	GLU .			16.858	20.187	40.721	1.00 25.84
MOTA	829	CA	GLU .			17.281	18.804	40.444	1.00 27.82
ATOM	830	С	GLU .			17.800	18.693	39.024	1.00 26.80
ATOM	831	0	GLU .			17.246	19.323	38.072	1.00 26.59
ATOM	832	CB	GLU .			16.121	17.834	40.678	1.00 31.67
ATOM	833	CG	GLU 3			16.233	17.118	42.020	1.00 38.94
ATOM	834	CD	GLU 2			14.913	16.568	42.519	1.00 41.54
ATOM	835	OE1				14.282	15.765	41.796	1.00 44.35
ATOM	836	OE2	GLU 2			14.510	16.940	43.644	1.00 43.84
ATOM	837	N	SER 2			18.861	17.919	38.852	1.00 24.81
ATOM	838	CA	SER I			19.455	17.765	37.525	1.00 25.32
ATOM	839	C	SER 2			20.213	16.459	37.397	1.00 25.44
ATOM	840	0	SER Z			20.551	15.795	38.427	1.00 24.00
ATOM	841	CB	SER Z			20.405	18.928	37.255	1.00 23.13
ATOM	842	OG	SER Z			21.444	18.939	38.217	1.00 21.22
ATOM	843	N	ASP A			20.490	16.079	36.155	1.00 26.01
MOTA	844	CA	ASP A			21.227	14.842	35.871	1.00 26.62
ATOM	845	С	ASP A			22.138	15.038	34.671	1.00 25.62
MOTA	846	0	ASP A			21.656	15.300	33.528	1.00 24.35
ATOM	847	CB	ASP A			20.253	13.691	35.601	1.00 30.53
MOTA	848	CG	ASP A			20.966	12.370	35.387	1.00 32.67
MOTA	849	OD1	ASP A	Α.	167	21.912	12.083	36.152	1.00 36.14
MOTA	850	OD2	ASP A	Α.	167	20.586	11.615	34.469	1.00 34.63
ATOM	851	N	LYS A	Α.	168	23.440	14.930	34.910	1.00 25.32
MOTA	852	CA	LYS A	A :	168	24.461	15.078	33.847	1.00 25.94
MOTA	853	C	LYS A	Α :	168	24.416	16.445	33.175	1.00 25.49
ATOM	854	0	LYS A	A :	168	24.742	16.580	31.955	1.00 25.50
MOTA	855	CB	LYS A	Α :	168	24.282	13.979	32.800	1.00 27.68
MOTA	856	CG	LYS 2	A .	168	24.408	12.570	33.362	1.00 30.33
MOTA	857	CD	LYS A			24.117	11.532	32.292	1.00 32.36
ATOM	858	CE	LYS A			24.205	10.126	32.855	1.00 34.37
ATOM	859	NZ	LYS A			23.889	9.101	31.821	1.00 36.50
MOTA	860	N	PHE A			24.024	17.460	33.937	1.00 22.87
MOTA	861	CA	PHE A			23.942	18.835	33.418	1.00 20.96
ATOM	862	С	PHE A			25.158	19.616	33.897	1.00 22.06
MOTA	863	0	PHE A			25.983	20.119	33.069	1.00 20.71
MOTA	864	CB	PHE A			22.668	19.506	33.919	1.00 19.76
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MOTA	865	CG	PHE A	169	22.526	20.931	33.479	1.00 18.95
ATOM	866	.CD1	PHE A	169	22.400	21.248	32.130	1.00 18.27
ATOM	867	CD2	PHE A	169	22.525	21.963	34.416	1.00 18.36
ATOM	868	CE1	PHE A	169	22.275	22.571	31.720	1.00 16.94
ATOM	869	CE2			22.401	23.287	34.013	1.00 17.25
ATOM	870	CZ	PHE A		22.275	23.590	32.661	1.00 16.89
ATOM	871	N	PHE A		25.292	19.738	35.212	1.00 20.46
ATOM	872	CA	PHE A		26.438	20.452	35.788	1.00 20.46
ATOM	873	C	PHE A		27.702	19.620		
ATOM	874	0	PHE A		27.702		35.574	1.00 22.40
ATOM	875	СВ				18.355	35.665	1.00 22.55
			PHE A		26.205	20.705	37.281	1.00 19.44
ATOM	876	CG	PHE A		25.079	21.663	37.559	1.00 18.44
ATOM	877		PHE A		23.988	21.276	38.330	1.00 18.45
ATOM	878		PHE A		25.098	22.948	37.025	1.00 16.73
ATOM	879	CE1	PHE A		22.932	22.154	38.563	1.00 17.50
MOTA	880	CE2	PHE A		24.046	23.832	37.253	1.00 17.78
ATOM	881	CZ	PHE A		22.963	23.432	38.023	1.00 16.39
ATOM	882	N	ILE A		28.805	20.297	35.272	1.00 23.10
MOTA	883	CA	ILE A	171	30.095	19.615	35.043	1.00 22.87
ATOM	884	С	ILE A	. 171	31.057	19.962	36.163	1.00 24.02
ATOM	885	0	ILE A	171	31.222	21.162	36.537	1.00 22.48
MOTA	886	CB	ILE A	171	30.729	20.048	33.704	1.00 24.70
MOTA	887	CG1	ILE A	171	29.823	19.632	32.544	1.00 22.57
MOTA	888	CG2	ILE A	*	32.123	19.434	33.558	1.00 22.35
ATOM	889	CD1	ILE A		30.319	20.100	31.192	1.00 23.46
ATOM	890	N	ASN A		31.702	18.942	36.709	1.00 27.12
ATOM	891	CA	ASN A		32.657	19.143	37.809	1.00 27.12
ATOM	892	C	ASN A		33.864	19.975	37.359	1.00 30.01
ATOM	893	ō	ASN A		34.616	19.574	36.418	1.00 29.20
ATOM	894	СВ	ASN A		33.105	17.779	38.337	
ATOM	895	CG	ASN A		33.913	17.885		1.00 31.92
ATOM	896		ASN A		33.615		39.608	1.00 34.74
ATOM	897	ND2	ASN A			18.737	40.504	1.00 36.04
ATOM	898	N N			34.927	17.034	39.734	1.00 36.14
ATOM	899		GLY A		34.049	21.132	37.991	1.00 28.24
		CA	GLY A		35.166	22.001	37.659	1.00 27.99
MOTA	900	С	GLY A		34.973	22.938	36.476	1.00 28.87
MOTA	901	0	GLY A		35.944	23.644	36.063	1.00 29.20
ATOM	902	N	SER A		33.769	22.988	35.914	1.00 28.95
MOTA	903	CA	SER A		33.498	23.880	34.748	1.00 29.13
MOTA	904	С	SER A		33.524	25.348	35.168	1.00 27.92
MOTA	905	0	SER A		33.878	26.255	34.354	1.00 29.51
ATOM	906	CB	SER A		32.130	23.562	34.148	1.00 28.90
MOTA	907	OG	SER A		31.102	23.922	35.054	1.00 30.49
MOTA	908	N	ASN A		33.140	25.593	36.416	1.00 25.45
MOTA	909	CA	ASN A		33.095	26.951	37.011	1.00 23.59
MOTA	910	С	ASN A		31.855	27.767	36.647	1.00 21.71
MOTA	911	0	ASN A		31.828	29.019	36.853	1.00 20.11
MOTA	912	CB	ASN A		34.354	27.754	36.662	1.00 27.01
MOTA	913	CG	ASN A		34.548	28.950	37.582	1.00 29.09
MOTA	914	OD1	ASN A	175	34.648	28.794	38.840	1.00 30.19
ATOM	915	ND2	ASN A	175	34.600	30.144	37.004	1.00 30.01
MOTA	916	N	TRP A	176	30.841	27.121	36.078	1.00 16.70
ATOM	917	CA	TRP A	176	29.590	27.847	35.790	1.00 18.41
ATOM	918	С	TRP A		28.482	27.170	36.580	1.00 17.87
MOTA	919	0	TRP A		28.534	25.927	36.838	1.00 15.45
ATOM	920	CB	TRP A		29.248	27.888	34.292	1.00 15.45
ATOM	921	CG	TRP A		29.257	26.588	33.563	1.00 10.40
MOTA	922		TRP A		30.291	26.063	32.842	1.00 17.33
ATOM	923		TRP A		28.165	25.668	33.425	1.00 17.33
ATOM	924		TRP A		29.911	24.881	32.258	1.00 17.78
ATOM	925		TRP A		28.612	24.613		
MOTA	926		TRP A		26.852	25.635	32.599	1.00 16.95
	- 2 0	223	u A	±,0 .	20.032	. 033	33.918	1.00 18.29

MOTA	927	CZ2	TRP A	176	27.794	23.532	32.252	1.00 17.40
ATOM	928	CZ3	TRP A	176	26.034	24.557	33.573	1.00 19.02
ATOM	929	CH2	TRP A		26.512	23.521	32.747	1.00 19.06
MOTA	930	N.	GLU A	. 177	27.496	27.950	37.005	1.00 18.68
MOTA	931	CA	GLU A	. 177	26.387	27.385	37.797	1.00 21.01
ATOM	932	С	GLU A	177	25.024	27.700	37.224	1.00 20.81
MOTA	933	0	GLU A		23.977	27.582	37.938	1.00 21.08
MOTA	934	CB	GLU A	. 177	26.461	27.869	39.250	1.00 22.84
ATOM	935	CG	GLU A	177	26.865	29.322	39.443	1.00 26.63
			GLU A					
ATOM	936	CD			28.377	29.531	39.446	1.00 27.90
MOTA	937	OE1	GLU A	. 177	29.121	28.568	39.726	1.00 28.44
MOTA	938	OE2	GLU A	177	28.818	30.670	39.186	1.00 28.24
ATOM	939	N	GLY A		25.007	28.088	35.953	1.00 18.48
ATOM	940	CA	GLY A		23.759	28.411	35.295	1.00 16.82
MOTA	941	С	GLY A	. 178	23.929	28.406	33.791	1.00 15.90
MOTA	942	0	GLY A	178	25.070	28.248	33.264	1.00 15.75
ATOM	943	N	ILE A		22.831	28.589	33.076	1.00 14.53
ATOM	944	CA	ILE A	. 179	22.882	28.588	31.610	1.00 14.26
ATOM	945	C	ILE A	179	22.007	29.701	31.057	1.00 14.53
MOTA	946	0	ILE A		20.896	29.980	31.603	1.00 15.23
MOTA	947	CB	ILE A		22.428	27.217	31.069	1.00 14.45
MOTA	948	CG1	ILE A	179	22.535	27.183	29.548	1.00 14.28
MOTA	949	CG2	ILE A	179	21.002	26.921	31.525	1.00 13.41
ATOM	950	CD1	ILE A		22.359	25.788	28.974	1.00 13.85
MOTA	951	N	LEU A		22.489	30.350	29.998	1.00 14.91
MOTA	952	CA	LEU A	180	21.763	31.464	29.353	1.00 14.24
MOTA	953	С	LEU A	180	21.311	31.050	27.961	1.00 15.19
ATOM	954	Ö.	LEU A					
					22.117	31.115	26.973	1.00 15.79
MOTA	955	CB	LEU A	180	22.675	32.690	29.223	1.00 14.83
MOTA	956	CG	LEU A	180	22.078	34.107	29.257	1.00 16.59
MOTA	957		LEU A		22.902	34.996	28.351	1.00 15.04
MOTA	958		LEU A		20.622	34.120	28.818	1.00 17.08
MOTA	959	N	GLY A	181	20.057	30.621	27.851	1.00 15.40
MOTA	960	CA	GLY A	181	19.525	30.227	26.561	1.00 13.68
ATOM	961	C	GLY A		19.276	31.481	25.741	1.00 15.03
MOTA	962	0	GLY A		18.402	32.330	26.107	1.00 14.58
ATOM	963	И.	LEU A	182	20.002	31.629	24.638	1.00 12.84
MOTA	964	CA	LEU A	182	19.859	32.831	23.787	1.00 13.53
MOTA	965	С	LEU A	182	19.029	32.646	22.521	1.00 14.25
MOTA	966	0	LEU A		18.883	33.607	21.701	1.00 13.52
ATOM	967	CB	LEU A	. 182	21.250	33.352	23.418	1.00 13.44
MOTA	968	CG	LEU A	182	22.036	33.949	24.583	1.00 11.84
ATOM	969	CD1	LEU A	182	23.506	34.067	24.211	1.00 11.17
ATOM	970		LEU A		21.450			
						35.311	24.936	1.00 12.14
MOTA	971	N	ALA A	183	18.491	31.449	22.322	1.00 15.12
MOTA	972	CA	ALA A	183	17.660	31.183	21.131	1.00 15.16
MOTA	973	С	ALA A		16.276	31.788	21.361	1.00 17.66
ATOM	974	Ō	ALA A		16.053			
						32.526	22.377	1.00 16.26
MOTA	975	CB	ALA A	. 183	17.557	29.684	20.875	1.00 14.23
MOTA	976	N	TYR A	184	15.338	31.487	20.466	1.00 18.41
MOTA	977	CA	TYR A		13.976	32.060	20.550	1.00 17.40
ATOM	978	С	TYR A		12.953	31.334	21.424	1.00 18.41
MOTA	979	0	TYR A	. 184	13.131	30.135	21.807	1.00 14.95
MOTA	980	CB	TYR A	184	13.411	32.237	19.138	1.00 18.07
ATOM	981	CG	TYR A		14.327	33.017	18.216	1.00 19.50
ATOM	982		TYR A		15.295	32.367	17.446	1.00 19.23
MOTA	983	CD2	TYR A	184	14.233	34.408	18.119	1.00 19.65
ATOM	984	CE1	TYR A	184	16.144	33.083	16.599	1.00 19.22
ATOM	985	CE2			15.079	35.134	17.279	1.00 19.50
ATOM	986	CZ	TYR A		16.027	34.466	16.521	1.00 19.86
ATOM	987	OH	TYR A	184	16.842	35.185	15.670	1.00 20.69
ATOM	987 988	OH N	TYR A		16.842 11.873	35.185 32.046	15.670 21.734	1.00 20.69 1.00 16.29

	000			405	40 804			
ATOM	989	CA	ALA A		10.784	31.519	22.592	1.00 17.90
MOTA	990	С	ALA A	185	10.185	30.221	22.068	1.00 17.38
ATOM	991	0	ALA A	185	9.682	29.372	22.869	1.00 15.41
MOTA	992	CB	ALA A	185	9.690	32.579	22.742	1.00 15.99
ATOM	993	N	GLU A		10.232	30.046	20.751	
								1.00 20.56
MOTA	994	CA	GLU A		9.679	28.846	20.086	1.00 23.43
ATOM	995	С	GLU A	186	10.169	27.533	20.690	1.00 23.87
MOTA	996	0	GLU A	186	9.448	26.486	20.619	1.00 24.67
ATOM	997	CB	GLU A	186	10.009	28.887	18.591	1.00 27.60
ATOM	998	CG	GLU A		9.447	27.729	17.786	1.00 32.42
		CD						
ATOM	999		GLU A		7.941	27.593	17.923	1.00 36.08
MOTA	1000	OE1			7.255	28.633	18.041	1.00 39.03
MOTA	1001	OE2	GLU A	186	7.439	26.448	17.900	1.00 37.05
MOTA	1002	N	ILE A	187	11.363	27.540	21.283	1.00 22.31
MOTA	1003	CA	ILE A	187	11.904	26.302	21.900	1.00 19.35
MOTA	1004	C	ILE A		12.113	26.441	23.403	1.00 20.13
		o						
MOTA	1005		ILE A		12.887	25.654	24.034	1.00 19.35
MOTA	1006	CB	ILE A		13.241	25.872	21.248	1.00 19.03
ATOM	1007	CG1	ILE A	187	14.270	26.998	21.355	1.00 18.36
MOTA	1008	CG2	ILE A	187	13.008	25.488	19.795	1.00 19.03
ATOM	1009	CD1	ILE A	187	15.627	26.635	20.780	1.00 17.45
ATOM	1010	N	ALA A		11.441	27.416	23.999	1.00 19.82
ATOM	1011	CA	ALA A					
					11.551	27.636	25.454	1.00 20.35
ATOM	1012	С	ALA A		10.622	26.661	26.171	1.00 19.60
ATOM	1013	0	ALA A		9.554	26.277	25.618	1.00 19.52
ATOM	1014	CB	ALA A	188	11.160	29.083	25.793	1.00 17.16
ATOM	1015	N	ARG A	189	11.004	26.231	27.372	1.00 20.77
ATOM	1016	CA	ARG A	189	10.142	25.324	28.164	1.00 21.43
ATOM	1017	С	ARG A		9.577	26.162	29.303	1.00 22.80
ATOM	1018	ō	ARG A		10.274			
						27.099	29.817	1.00 23.68
MOTA	1019	СВ	ARG A		10.949	24.151	28.753	1.00 22.36
MOTA	1020	CG	ARG A		11.689	23.285	27.729	1.00 23.90
ATOM	1021	CD	ARG A	189	10.765	22.818	26.624	1.00 24.33
MOTA	1022	NE	ARG A	189	11.419	21.914	25.681	1.00 25.35
MOTA	1023	CZ	ARG A	189	11.336	20.586	25.724	1.00 27.35
MOTA	1024	NH1	ARG A			19.991	26.673	1.00 24.73
ATOM	1025	NH2	ARG A		11.959	19.849	24.807	1.00 25.42
ATOM	1026		PRO A					
		N			8.325	25.890	29.725	1.00 23.27
ATOM	1027	CA	PRO A		7.442	24.830	29.216	1.00 23.21
ATOM	1028	С	PRO A		6.826	25.110	27.849	1.00 23.72
ATOM	1029	0	PRO A	190	6.458	24.157	27.101	1.00 23.77
MOTA	1030	CB	PRO A	190	6.377	24.713	30.305	1.00 22.63
MOTA	1031	CG	PRO A	190	6.285	26.115	30.830	1.00 24.33
MOTA	1032	CD	PRO A		7.745	26.527	30.921	1.00 22.73
ATOM	1033	N	ASP A		6.681	26.383		
							27.508	1.00 25.20
ATOM	1034	CA	ASP A		6.107	26.754	26.202	1.00 25.89
MOTA	1035	C	ASP A		6.653	28.106	25.770	1.00 25.76
MOTA	1036	0	ASP A	191	7.488	28.716	26.498	1.00 24.40
MOTA	1037	CB	ASP A	191	4.569	26.757	26.269	1.00 28.36
MOTA	1038	CG	ASP A	191	4.024	27.697	27.323	1.00 30.16
MOTA	1039		ASP A		2.887	27.468	27.783	1.00 33.88
MOTA	1040		ASP A		4.714			1.00 30.53
ATOM	1040					28.669	27.686	
		N	ASP A		6.214	28.596	24.617	1.00 26.01
MOTA	1042	CA	ASP A		6.724	29.877	24.088	1.00 26.22
MOTA	1043	С	ASP A		6.236	31.123	24.813	1.00 26.52
MOTA	1044	0	ASP A	192	6.567	32.275	24.395	1.00 26.27
MOTA	1045	СВ	ASP A		6.419	29.985	22.589	1.00 27.69
MOTA	1046	CG	ASP A		4.940	30.161	22.296	1.00 29.61
MOTA	1047		ASP A		4.102	29.647	23.066	1.00 31.87
MOTA	1048		ASP A		4.618			1.00 31.87
ATOM	1049					30.805	21.279	
		N	SER A		5.470	30.947	25.885	1.00 24.46
MOTA	1050	CA	SER A	193	4.988	32.117	26.645	1.00 24.21
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MOTA	1051	С	SER A 193	6.078	32.565	27.614	1.00 22.68
MOTA	1052	0	SER A 193	6.082	33.740	28.082	1.00 22.41
ATOM	1053	CB	SER A 193	3.701	31.787	27.415	1.00 25.67
ATOM	1054	OG	SER A 193		30.774	28.386	1.00 27.13
ATOM	1055	N	LEU A 194		31.670	27.932	1.00 20.84
MOTA	1056	CA	LEU A 194		32.044		
						28.852	1.00 18.87
ATOM	1057	C	LEU A 194		32.830	28.065	1.00 18.82
MOTA	1058	0	LEU A 194		32.240	27.419	1.00 19.19
ATOM	1059	СВ	LEU A 194	8.758	30.809	29.469	1.00 17.48
ATOM	1060	CG	LEU A 194		31.201	30.631	1.00 19.18
MOTA	1061	CD1	LEU A 194	8.825	31.633	31.825	1.00 16.80
MOTA	1062	CD2	LEU A 194	10.585	30.044	31.014	1.00 16.32
MOTA	1063	N	GLU A 195		34.150	28.095	1.00 18.44
ATOM	1064	CA	GLU A 195		35.029	27.369	1.00 18.80
ATOM	1065	C	GLU A 195		34.777	27.733	
ATOM	1066	Ö	GLU A 195				1.00 19.02
					34.754	28.953	1.00 17.72
ATOM	1067	CB	GLU A 195		36.485	27.644	1.00 20.83
ATOM	1068	CG	GLU A 195		37.512	27.047	1.00 23.03
ATOM	1069	CD	GLU A 195		38.926	27.204	1.00 24.10
MOTA	1070	OE1			39.373	26.337	1.00 25.77
ATOM	1071	OE2	GLU A 195	10.343	39.585	28.203	1.00 24.06
ATOM	1072	N	PRO A 196	12.272	34.559	26.714	1.00 18.43
ATOM	1073	CA	PRO A 196	13.702	34.311	26.935	1.00 18.17
ATOM	1074	С	PRO A 196		35.571	27.447	1.00 16.90
ATOM	1075	0	PRO A 196		36.715	27.297	1.00 17.67
ATOM	1076	СВ	PRO A 196		33.914	25.546	1.00 17.07
MOTA	1077	CG	PRO A 196				
ATOM	1077				33.305	24.892	1.00 19.11
		CD	PRO A 196		34.287	25.310	1.00 18.58
ATOM	1079	И	PHE A 197		35.405	28.039	1.00 15.80
ATOM	1080	CA	PHE A 197		36.550	28.574	1.00 14.47
ATOM	1081	С	PHE A 197		37.663	27.576	1.00 16.31
MOTA	1082	О	PHE A 197		38.873	27.894	1.00 14.87
ATOM	1083	CB	PHE A 197	17.595	36.093	29.217	1.00 12.99
MOTA	1084	CG	PHE A 197	18.472	37.227	29.652	1.00 13.09
MOTA	1085	CD1	PHE A 197		37.806	28.767	1.00 12.33
ATOM	1086	CD2	PHE A 197	18.347	37.766	30.926	1.00 14.29
MOTA	1087	CE1	PHE A 197	20.139	38.907	29.143	1.00 12.22
MOTA	1088	CE2	PHE A 197	19.108	38.873	31.310	1.00 14.64
ATOM	1089	CZ	PHE A 197	20.002	39.441	30.415	1.00 13.26
MOTA	1090	N	PHE A 198	17.089	37.319	26.390	1.00 16.71
ATOM	1091	CA	PHE A 198		38.384	25.431	1.00 17.60
MOTA	1092	С	PHE A 198		39.192	25.001	1.00 17.52
MOTA	1093	0	PHE A 198	16.317	40.434	24.774	1.00 16.03
ATOM	1094	CB	PHE A 198		37.829	24.196	1.00 17.77
ATOM	1095	CG	PHE A 198		38.826	23.549	1.00 17.77
ATOM	1096		PHE A 198		39.075	24.087	
ATOM	1097		PHE A 198				1.00 18.66
ATOM	1098				39.569	22.455	1.00 16.90
ATOM			PHE A 198	21.139	40.053	23.546	1.00 18.55
	1099		PHE A 198	19.454	40.551	21.904	1.00 17.96
ATOM	1100	CZ	PHE A 198	20.708	40.795	22.451	1.00 18.52
MOTA	1101	N	ASP A 199		38.530	24.879	1.00 17.52
ATOM	1102	CA	ASP A 199	13.819	39.225	24.491	1.00 19.54
ATOM	1103	С	ASP A 199	13.464	40.261	25.561	1.00 18.83
MOTA	1104	0	ASP A 199	13.134	41.444	25.233	1.00 20.48
ATOM	1105	CB	ASP A 199	12.685	38.210	24.338	1.00 21.95
ATOM	1106	CG	ASP A 199	12.868	37.312	23.126	1.00 24.77
MOTA	1107	0D1	ASP A 199	12.408	37.687	22.028	1.00 27.27
ATOM	1108	OD2	ASP A 199	13.481	36.234	23.261	1.00 27.11
MOTA	1109	N	SER A 200	13.530	39.858	26.829	1.00 17.89
MOTA	1110	CA	SER A 200	13.223	40.784	27.947	1.00 16.17
MOTA	1111	С	SER A 200	14.211	41.943	27.915	1.00 16.77
MOTA	1112	0	SER A 200	13.823	43.140	28.072	1.00 17.20

MOTA	1113	CB	SER A	200	13.336	40.062	29.292	1.00 14.55
ATOM	1114	OG	SER A	200	12.386	39.017	29.400	1.00 14.16
ATOM	1115	N	LEU A	201	15.481	41.617	27.711	1.00 16.47
ATOM	1116	CA	LEU A		16.553	42.638	27.654	1.00 18.93
MOTA	1117	С	LEU A	201	16.237	43.684	26.586	1.00 18.88
ATOM	1118	0	LEU A	201	16.274	44.917	26.852	1.00 18.26
MOTA	1119	СВ	LEU A		17.884	41.953	27.337	1.00 18.68
ATOM	1120	CG	LEU A		19.244	42.637	27.523	1.00 20.59
ATOM	1121		LEU A		19.973		26.194	1.00 20.98
ATOM	1122		LEU A		19.100	44.053	28.045	1.00 20.13
ATOM	1123	N	VAL A		15.919	43.222	25.383	1.00 20.38
ATOM	1124	CA	VAL A		15.600	44.130	24.264	1.00 20.23
ATOM	1125	C	VAL A		14.335	44.938	24.532	1.00 23.13
MOTA	1126	0	VAL A		14.284	46.175	24.255	1.00 23.36
ATOM	1127	СВ	VAL A		15.433	43.337	22.948	1.00 19.84
ATOM	1128		VAL A		14.830	44.228	21.855	1.00 17.60
ATOM	1129		VAL A		16.792	42.804	22.502	1.00 16.36
ATOM	1130	N	LYS A		13.315	44.285	25.074	1.00 24.15
ATOM	1131	CA	LYS A		12.050	44.985	25.360	1.00 27.77
ATOM	1132	C	LYS A		12.178	46.049	26.452	1.00 27.47
ATOM	1133	Ō	LYS A		11.753	47.223	26.252	1.00 26.63
ATOM	1134	ČВ	LYS A		10.970	43.973	25.746	1.00 29.55
ATOM	1135	CG	LYS A		9.609	44.594	26.008	1.00 34.08
ATOM	1136	CD	LYS A		8.497	43.798	25.335	1.00 34.00
ATOM	1137	CE	LYS A		8.504	42.342	25.774	1.00 38.97
ATOM	1138	NZ	LYS A		7.512	41.533	25.012	1.00 40.86
ATOM	1139	N	GLN A		12.771	45.687	27.585	1.00 26.46
ATOM	1140	CA			12.910	46.632	28.721	1.00 26.94
ATOM	1141	C	GLN A		14.125	47.542	28.614	1.00 28.51
ATOM	1142	ō	GLN A		14.479	48.264	29.600	1.00 30.36
ATOM	1143	CB	GLN A		13.007	45.848	30.032	1.00 24.17
ATOM	1144	CG	GLN A		11.980	44.739	30.170	1.00 20.78
ATOM	1145	CD	GLN A		12.270	43.821	31.342	1.00 20.14
ATOM	1146		GLN A		11.725	42.676	31.420	1.00 19.72
ATOM	1147	NE2	GLN A		13.107	44.279	32.265	1.00 16.56
ATOM	1148	N	THR A		14.762	47.568	27.453	1.00 28.58
ATOM	1149	CA	THR A		15.979	48.375	27.306	1.00 29.06
ATOM	1150	С	THR A		16.186	48.905	25.885	1.00 30.58
ATOM	1151	Ō	THR A		15.427	48.525	24.940	1.00 30.23
MOTA	1152	CB	THR A		17.175	47.501	27.772	1.00 29.85
ATOM	1153	OG1			17.572	47.899	29.088	1.00 29.62
MOTA	1154	CG2	THR A	205	18.328	47.576	26.823	1.00 29.03
MOTA	1155	N	HIS A		17.175	49.784		1.00 31.92
ATOM	1156	CA	HIS A		17.488	50.350	24.372	1.00 33.38
MOTA	1157	С	HIS A		18.548	49.530	23.637	1.00 32.31
MOTA	1158	0	HIS A	206	18.905	49.845	22.460	1.00 31.08
ATOM	1159	СВ	HIS A	206	17.975	51.799	24.487	1.00 36.39
MOTA	1160	CG	HIS A	206	16.898	52.773	24.848	1.00 39.92
MOTA	1161	ND1	HIS A		15.696	52.836	24.177	1.00 40.95
ATOM	1162	CD2	HIS A	206	16.849	53.736	25.800	1.00 40.35
MOTA	1163	CE1	HIS A	206	14.951	53.794	24.699	1.00 41.58
MOTA	1164	NE2	HIS A	206	15.627	54.356	25.685	1.00 41.65
MOTA	1165	N	VAL A	207	19.075	48.501	24.291	1.00 29.55
MOTA	1166	CA	VAL A	207	20.097	47.639	23.651	1.00 28.49
MOTA	1167	С	VAL A	207	19.511	47.083	22.354	1.00 26.27
MOTA	1168	0	VAL A	207	18.415	46.441	22.358	1.00 26.26
MOTA	1169	CB	VAL A	207	20.498	46.462	24.572	1.00 28.77
MOTA	1170	CG1	VAL A	207	21.399	45.491	23.825	1.00 29.45
MOTA	1171	CG2	VAL A	207	21.219	46.987	25.805	1.00 28.52
MOTA	1172	N	PRO A		20.192	47.311	21.220	1.00 24.42
MOTA	1173	CA	PRO A		19.683	46.804	19.944	1.00 23.82
MOTA	1174	С	PRO A	208	19.547	45.284	19.914	1.00 22.81

ATOM	1175	0	PRO A	208	2	0.290	44.545	20.630	1.00 21.12
MOTA	1176	CB	PRO A	208	2	0.689	47.343	18.926	1.00 24.65
MOTA	1177	CG	PRO A	208	2	1.927	47.510	19.711	1.00 25.77
MOTA	1178	CD	PRO A	208	2	1.441	48.062	21.025	1.00 24.39
ATOM	1179	N	ASN A	209	1	8.605	44.806	19.109	1.00 21.59
MOTA	1180	CA	ASN A	209	1	8.322	43.362	18.995	1.00 20.43
ATOM	1181	С	ASN A	209	1	9.390	42.599	18.222	1.00 20.52
ATOM	1182	0	ASN A	209	1	9.190	42.217	17.026	1.00 21.39
ATOM	1183	CB	ASN A		1	6.957	43.159	18.340	1.00 18.52
ATOM	1184	CG	ASN A			6.501	41.728	18.402	1.00 18.12
ATOM	1185		ASN A			6.968	40.948	19.281	1.00 18.32
ATOM	1186		ASN A			5.594	41.348	17.513	1.00 15.63
ATOM	1187	N	LEU A			0.514	42.346	18.883	1.00 19.53
ATOM	1188	CA	LEU A			1.631	41.634	18.243	1.00 19.83
ATOM	1189	C	LEU A			2.765	41.421	19.226	1.00 19.02
	1190		LEU A			2.958	42.238	20.176	1.00 18.52
MOTA		0	LEU A			2.120	42.451	17.035	1.00 21.93
MOTA	1191	CB				3.534	42.305	16.456	1.00 21.35
MOTA	1192	CG	LEU A						
MOTA	1193		LEU A			3.612	43.009	15.102	1.00 23.20
ATOM	1194		LEU A			4.548	42.910	17.409	1.00 24.60
MOTA	1195	N	PHE A			3.509	40.334	19.044	1.00 16.48
MOTA	1196	CA	PHE A			4.671	40.055	19.909	1.00 16.70
MOTA	1197	С	PHE A			5.722	39.310	19.095	1.00 16.08
MOTA	1198	0	PHE A			5.392	38.653	18.063	1.00 17.22
MOTA	1199	CB	PHE A			4.251	39.280	21.173	1.00 14.67
MOTA	1200	CG		1 211		3.813	37.863	20.924	1.00 16.01
MOTA	1201	CD1				4.748	36.837	20.835	1.00 14.91
MOTA	1202	CD2	PHE A			2.465	37.546	20.824	1.00 14.62
MOTA	1203	CE1	PHE A		2	4.344	35.515	20.653	1.00 15.05
MOTA	1204	CE2	PHE A	1 211	2	2.054	36.224	20.641	1.00 15.47
MOTA	1205	CZ	PHE A	211		2.996	35.207	20.558	1.00 12.73
MOTA	1206	N	SER A	1 212	2	6.977	39.424	19.520	1.00 17.19
MOTA	1207	CA	SER 7	1 212	2	8.126	38.803	18.818	1.00 16.98
MOTA	1208	С	SER A	A 212	2	8.894	37.862	19.725	1.00 16.10
ATOM \	1209	0	SER A	A 212	2	9.036	38.122	20.955	1.00 14.22
MOTA	1210	CB	SER A	A 212	2	9.094	39.888	18.349	1.00 16.89
MOTA	1211	OG	SER A	A 212	2	8.431	40.869	17.593	1.00 26.70
MOTA	1212	N	LEU A	A 213	2	9.430	36.797	19.144	1.00 14.76
MOTA	1213	CA	LEU A	A 213	3	0.194	35.819	19.930	1.00 14.81
MOTA	1214	C	LEU A	A 213	3	1.563	35.509	19.352	1.00 14.32
MOTA	1215	0	LEU A	A 213	3	1.702	35.162	18.137	1.00 12.74
MOTA	1216	CB	LEU A	A 213	2	9.394	34.522	20.060	1.00 15.67
MOTA	1217	CG	LEU A	A 213	2	8.735	34.210	21.408	1.00 18.95
MOTA	1218	CD1	LEU A	A 213	2	8.196	35.475	22.050	1.00 18.65
MOTA	1219	CD2	LEU A	A 213	2	7.627	33.185	21.192	1.00 16.46
MOTA	1220	N	GLN A	A 214	3	2.581	35.656	20.191	1.00 14.19
ATOM	1221	CA	GLN A	A 214	3	3.954	35.324	19.797	1.00 15.89
MOTA	1222	С	GLN Z	A 214	3	4.407	34.258	20.778	1.00 15.04
MOTA	1223	0	GLN A	A 214	3	4.848	34.582	21.917	1.00 16.01
MOTA	1224	CB	GLN A	A 214	. 3	4.903	36.523	19.914	1.00 17.92
MOTA	1225	CG	GLN A	A 214	3	6.290	36.231	19.341	1.00 20.63
MOTA	1226	CD		A 214		7.397	37.099	19.932	1.00 23.22
ATOM	1227		GLN A	A 214		8.459	37.332	19.273	1.00 24.79
MOTA	1228	NE2		A 214		7.199	37.571	21.156	1.00 24.53
MOTA	1229	N		A 215		4.284	32.997	20.390	1.00 14.37
MOTA	1230	CA		A 215		4.729	31.890		1.00 13.74
MOTA	1231	С		A 215		6.193	31.625	20.925	1.00 14.40
ATOM	1232	Ō		A 215		6.541	31.357	19.737	1.00 14.39
ATOM	1233	СВ		A 215		3.872	30.644	21.005	1.00 13.94
ATOM	1234	CG		A 215		2.636	30.429	21.893	1.00 14.78
MOTA	1235		LEU A			1.900	31.734	22.143	1.00 13.31
MOTA	1236		LEU			1.723	29.407	21.240	1.00 12.97
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3.000	1007			016	20 000	34 506	04 000	1 00 14 00
MOTA	1237	N	CYS A		37.066	31.706	21.922	1.00 14.83
MOTA	1238	CA	CYS A	216	38.504	31.486	21.682	1.00 16.37
ATOM	1239	С	CYS A	216	39.066	30.196	22.263	1.00 17.20
ATOM	1240	0	CYS A		39.174	30.046	23.519	1.00 16.79
MOTA	1241	CB	CYS A		39.314	32.668	22.227	1.00 19.03
ATOM	1242	SG	CYS A	216	38.852	34.278	21.505	1.00 23.75
MOTA	1243	N	GLY A	217	39.415	29.257	21.387	1.00 15.43
ATOM	1244	CA	GLY A		40.018	28.021	21.843	
								1.00 16.40
MOTA	1245	C	GLY A		41.483	28.371	22.064	1.00 17.87
MOTA	1246	0	GLY A	217	42.057	29.204	21.303	1.00 17.53
ATOM	1247	N	ALA A	218	42.119	27.785	23.069	1.00 17.79
ATOM	1248	CA	ALA A		43.539	28.108	23.349	1.00 16.33
MOTA	1249	С	ALA A		44.486	27.408	22.379	1.00 17.71
MOTA	1250	0	ALA A	218	45.602	27.927	22.069	1.00 16.46
ATOM	1251	CB	ALA A	218	43.884	27.731	24.779	1.00 14.95
ATOM	1252	N	GLY A		44.073	26.245	21.890	1.00 16.19
ATOM	1253	CA	GLY A		44.909	25.505	20.970	1.00 17.57
MOTA	1254	С	GLY A	219	45.696	24.439	21.703	1.00 17.52
ATOM	1255	0	GLY A	219	46.490	23.675	21.076	1.00 16.29
MOTA	1256	N	PHE A	220	45.502	24.375	23.018	1.00 17.13
ATOM	1257							
		CA	PHE A		46.190	23.381	23.873	1.00 18.29
MOTA	1258	С	PHE A		45.381	23.185	25.153	1.00 19.24
MOTA	1259	0	PHE A	220	44.477	24.012	25.475	1.00 19.69
ATOM	1260	CB	PHE A	220	47.616	23.854	24.187	1.00 18.72
MOTA	1261	CG	PHE A		47.689	25.253	24.731	1.00 20.07
MOTA	1262		PHE A		47.448	25.507	26.077	1.00 20.91
MOTA	1263	CD2	PHE A	220	47.984	26.320	23.890	1.00 19.91
ATOM	1264	CE1	PHE A	220	47.505	26.809	26.576	1.00 21.79
ATOM	1265	CE2	PHE A	220	48.043	27.620	24.374	1.00 20.35
ATOM	1266	CZ	PHE A		47.802	27.866	25.721	1.00 21.77
ATOM	1267	N	PRO A		45.659	22.110	25.907	1.00 20.17
MOTA	1268	CA	PRO A	221	44.922	21.846	27.147	1.00 21.27
MOTA	1269	С	PRO A	221	45.014	22.959	28.180	1.00 23.04
MOTA	1270	0	PRO A	221	46.065	23.666	28.292	1.00 23.99
MOTA	1271	СВ	PRO A		45.545	20.543	27.648	1.00 20.22
ATOM	1272	CG	PRO A		45.946	19.855	26.390	1.00 20.63
MOTA	1273	CD	PRO A		46.571	20.994	25.602	1.00 20.45
MOTA	1274	N	LEU A	222	43.934	23.132	28.933	1.00 25.72
MOTA	1275	CA	LEU A	222	43.873	24.158	29.991	1.00 28.32
ATOM	1276	С	LEU A	222	43.425	23.516	31.291	1.00 30.88
MOTA	1277	0	LEU A	222	42.248	23.042	31.403	1.00 31.71
ATOM	1278	СВ	LEU A		42.880	25.261	29.620	
								1.00 27.52
MOTA	1279	CG			43.264		28.506	1.00 27.30
MOTA	1280		LEU A		42.040	27.042	28.096	1.00 26.79
MOTA	1281	CD2	LEU A	222	44.382	27.143	28.983	1.00 27.13
MOTA	1282	N	ASN A	223	44.320	23.470	32.273	1.00 34.15
MOTA	1283	CA	ASN A		43.959	22.893	33.583	1.00 37.64
MOTA	1284	С	ASN A		43.014	23.882	34.254	1.00 38.54
MOTA	1285	0	ASN A	223	42.864	25.056	33.785	1.00 36.72
MOTA	1286	CB	ASN A	223	45.204	22.663	34.457	1.00 38.54
MOTA	1287	CG	ASN A	223	45.905		34.839	1.00 39.09
ATOM	1288		ASN A		45.268		35.375	1.00 41.39
ATOM	1289		ASN A		47.208		34.595	1.00 40.09
ATOM	1290	N	GLN A		42.380	23.444	35.335	1.00 41.79
MOTA	1291	CA	GLN A	224	41.415	24.278	36.073	1.00 43.58
MOTA	1292	С	GLN A	224	41.898		36.359	1.00 42.52
ATOM	1293	0	GLN A		41.138		36.126	1.00 42.75
ATOM	1294	СВ	GLN A					
					41.021	23.572	37.378	1.00 46.22
ATOM	1295	CG	GLN A		39.629		37.827	1.00 49.86
ATOM	1296	CD	GLN A		39.085	23.160	38.990	1.00 51.40
MOTA	1297		GLN A		37.923	23.406	39.443	1.00 52.42
MOTA	1298	NE2	GLN A	224	39.866	22.215	39.496	1.00 52.75
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MOTA	1299	N	SER			43.133	25.852	36.831	1.00 40.27
ATOM	1300	CA	SER	Α	225	43.669	27.200	37.138	1.00 39.30
MOTA	1301	С	SER	Α	225	43.989	28.028	35.893	1.00 36.57
MOTA	1302	0	SER	Α	225	43.920	29.292	35.930	1.00 36.27
ATOM	1303	CB	SER	Α	225	44.917	27.094	38.027	1.00 40.27
MOTA	1304	OG	SER	Α	225	45.974	26.411	37.376	1.00 42.21
ATOM	1305	N	GLU	Α	226	44.339	27.364	34.796	1.00 34.29
ATOM	1306	CA	GLU	Α	226	44.654	28.083	33.542	1.00 32.79
ATOM	1307	С	GLU	Α	226	43.375	28.651	32.954	1.00 31.17
ATOM	1308	0	GLU	Α	226	43.354	29.815	32.454	1.00 29.09
ATOM	1309	СВ	GLU	Α	226	45.307	27.144	32.526	1.00 33.69
ATOM	1310	CG	GLU			46.708	26.696	32.902	1.00 36.40
ATOM	1311	CD	GLU			47.251	25.619	31.972	1.00 37.70
ATOM	1312		GLU			46.585	24.567	31.830	1.00 37.54
ATOM	1313		GLU			48.340	25.823	31.389	1.00 37.14
ATOM	1314	N	VAL			42.305	27.867	33.007	1.00 29.89
ATOM	1315	CA	VAL			41.013	28.312	32.458	1.00 30.15
MOTA	1316	C	VAL			40.512	29.547	33.203	1.00 29.84
ATOM	1317	0	VAL			39.922	30.484	32.582	1.00 30.30
ATOM	1318	CB	VAL			39.940	27.210	32.558	1.00 30.93
ATOM	1319		VAL			38.800	27.538	31.637	1.00 30.53
	1320		VAL			40.516	25.867	32.183	1.00 32.07
ATOM						40.731			1.00 28.88
ATOM ATOM	1321	N CA	LEU LEU				29.581 30.726	34.513 35.336	1.00 28.88
	1322					40.292		34.975	
ATOM	1323	C	LEU			41.059	31.992		1.00 27.59
MOTA	1324	0	LEU			40.491	33.129	35.020	1.00 27.84
ATOM	1325	CB	LEU			40.496	30.420	36.819	1.00 27.50
MOTA	1326	CG	LEU			39.700	29.259	37.419	1.00 29.32
MOTA	1327		LEU			40.129	29.053	38.867	1.00 28.16
ATOM	1328		LEU			38.205	29.549	37.339	1.00 28.58
ATOM	1329	N	ALA			42.327	31.835	34.610	1.00 27.12
MOTA	1330	CA	ALA			43.176	32.998	34.257	1.00 27.64
ATOM	1331	С	ALA			43.134	33.347	32.776	1.00 27.65
MOTA	1332	0	ALA			43.460	34.504	32.375	1.00 29.94
ATOM	1333	СВ	ALA			44.617	32.736	34.682	1.00 27.52
ATOM	1334	N			230	42.736	32.393	31.947	1.00 26.68
MOTA	1335	CA	SER			42.692	32.635	30.498	1.00 26.33
MOTA	1336	С	SER			41.438	33.360	30.032	1.00 26.22
MOTA	1337	0	SER			40.356	33.302	30.695	1.00 25.70
MOTA	1338	CB			230	42.815	31.310	29.746	1.00 26.07
ATOM	1339	OG			230	42.759	31.519	28.344	1.00 26.54
ATOM	1340	N	VAL			41.562	34.056	28.909	1.00 25.03
MOTA	1341	CA	VAL			40.415	34.764	28.320	1.00 24.89
MOTA	1342	C	VAL			39.785	33.776	27.346	1.00 24.75
MOTA	1343	0	VAL			40.453	33.310	26.371	1.00 25.97
ATOM	1344	CB	VAL			40.859	36.043	27.568	1.00 24.38
MOTA	1345		VAL			39.729	36.554	26.678	1.00 22.98
MOTA	1346		VAL			41.244	37.119	28.577	1.00 23.20
MOTA	1347	N	GLY			38.526	33.433	27.588	1.00 23.26
MOTA	1348	CA	GLY			37.846	32.481	26.729	1.00 22.77
MOTA	1349	С	GLY			37.125	33.081	25.538	1.00 21.57
MOTA	1350	0	GLY			36.590	32.324	24.666	1.00 20.69
MOTA	1351	N	GLY			37.078	34.408	25.468	1.00 19.21
MOTA	1352	CA	GLY			36.410	35.050	24.353	1.00 17.96
MOTA	1353	С	GLY			35.599	36.275	24.731	1.00 18.25
MOTA	1354	0	GLY			35.778	36.866	25.851	1.00 15.19
MOTA	1355	N			234	34.708	36.677	23.828	1.00 16.58
MOTA	1356	CA	SER	A	234	33.864	37.864	24.053	1.00 16.83
MOTA	1357	С	SER	A	234	32.423	37.667	23.599	1.00 17.82
MOTA	1358	0	SER	A	234	32.134	36.995	22.552	1.00 17.90
MOTA	1359	СВ	SER	A	234	34.426	39.072	23.291	1.00 16.36
MOTA	1360	OG	SER	Α	234	35.816	39.253	23.508	1.00 18.23
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ATOM	1361	N	MET I	A 235	31.506	38.227	24.372	1.00 18.00
MOTA	1362	CA	MET A	A 235	30.091	38.201	24.010	1.00 17.58
ATOM	1363	C	MET Z	A 235	29.732	39.677	23.996	1.00 18.27
MOTA	1364	0	MET A	A 235	29.594	40.322	25.087	1.00 19.03
ATOM	1365	СВ	MET 2	A 235	29.232	37.475	25.046	1.00 16.91
ATOM	1366	CG		A 235	27.759	37.455	24.634	1.00 17.60
ATOM	1367	SD		A 235	26.597	36.751	25.819	
								1.00 20.56
MOTA	1368	CE		235	25.105	36.803	24.857	1.00 21.69
MOTA	1369	N		A 236	29.629	40.248	22.801	1.00 19.70
MOTA	1370	CA		¥ 236	29.271	41.669	22.674	1.00 19.40
MOTA	1371	С	ILE A	A 236	27.764	41.758	22.522	1.00 20.06
ATOM	1372	0	ILE A	A 236	27.175	41.365	21.467	1.00 16.87
ATOM	1373	CB	ILE A	A 236	29.985	42.341	21.470	1.00 21.41
MOTA	1374	CG1	ILE 2	A 236	31.452	42.625	21.821	1.00 22.57
MOTA	1375	CG2	ILE 2	A 236	29.329	43.672	21.149	1.00 21.72
ATOM	1376	CD1	ILE A	A 236	32.243	41.426	22.228	1.00 25.65
ATOM	1377	N	ILE 2	A 237	27.122	42.246	23.575	1.00 20.16
ATOM	1378	CA		A 237	25.663	42.382	23.599	1.00 21.01
MOTA	1379	C		A 237	25.215	43.710	22.996	1.00 22.16
ATOM	1380	ō		A 237	25.620	44.812	23.472	1.00 22.10
ATOM	1381	CB		A 237	25.153	42.241	25.050	1.00 22.36
ATOM	1382	CG1		A 237	25.346	40.791	25.498	1.00 22.29
MOTA	1383	CG2		A 237	23.694	42.660	25.156	1.00 20.45
MOTA	1384	CD1		A 237	25.002	40.529	26.939	1.00 24.84
MOTA	1385	N		A 238	24.404	43.626	21.946	1.00 23.30
ATOM	1386	CA	GLY 2	4 238	23.903	44.820	21.288	1.00 25.11
MOTA	1387	С	GLY 2	A 238	24.821	45.437	20.244	1.00 26.35
ATOM	1388	0	GLY 2	A 238	24.644	46.640	19.874	1.00 27.08
ATOM	1389	N	GLY 2	A 239	25.792	44.681	19.743	1.00 25.50
ATOM	1390	CA	GLY 2	A 239	26.679	45.251	18.747	1.00 24.81
ATOM	1391	С	GLY Z	A 239	27.807	44.371	18.242	1.00 26.38
MOTA	1392	0		A 239	27.942	43.167	18.632	1.00 23.61
MOTA	1393	N		A 240	28.632	44.960	17.383	1.00 26.33
ATOM	1394	CA		A 240	29.780	44.273	16.758	1.00 25.87
ATOM	1395	C		A 240	31.067	45.033	17.055	1.00 26.95
ATOM	1396	Ö		A 240	31.121	46.287	16.882	
MOTA	1397							1.00 28.86
		CB		A 240	29.607	44.226	15.226	1.00 25.88
ATOM	1398	CG1		4 240	28.298	43.519	14.871	1.00 25.12
ATOM	1399	CG2		A 240	30.806	43.541	14.581	1.00 26.56
ATOM	1400	CD1		A 240	27.939	43.599	13.396	1.00 24.59
MOTA	1401	N		A 241	32.100	44.323	17.498	1.00 25.24
MOTA	1402	CA	ASP .	A 241	33.395	44.973	17.781	1.00 25.13
MOTA	1403	С		A 241	34.383	44.548	16.698	1.00 26.31
MOTA	1404	0		A 241	34.676	43.326	16.536	1.00 26.89
ATOM	1405	CB	ASP .	A 241	33.922	44.561	19.153	1.00 24.85
MOTA	1406	CG	ASP .	A 241	35.171	45.325	19.541	1.00 24.81
ATOM	1407	OD1	ASP .	A 241	35.144	46.032	20.567	1.00 27.86
MOTA	1408	OD2	ASP .	A 241	36.180	45.226	18.817	1.00 25.69
MOTA	1409	N	HIS I	A 242	34.913	45.517	15.960	1.00 26.86
ATOM	1410	CA	HIS .	A 242	35.853	45.222	14.852	1.00 27.45
ATOM	1411	С		A 242	37.197	44.613	15.221	1.00 25.41
ATOM	1412	0		A 242	37.871	43.998	14.347	1.00 23.94
ATOM	1413	СВ		A 242	36.085	46.481	14.013	1.00 32.38
ATOM	1414	CG		A 242	34.858	46.957	13.304	1.00 37.46
ATOM	1415		HIS		33.822	47.591		
ATOM	1416		HIS .				13.956	1.00 39.65
	1417				34.472	46.837	12.011	1.00 39.29
ATOM			HIS.		32.850	47.840	13.096	1.00 40.56
MOTA	1418		HIS .		33.219	47.392	11.909	1.00 40.36
ATOM	1419	N		A 243	37.615	44.751	16.471	1.00 22.23
MOTA	1420	CA		A 243	38.915	44.184	16.877	1.00 22.06
ATOM	1421	C		A 243	38.843	42.667	17.011	1.00 20.51
MOTA	1422	0	SER .	A 243	39.897	41.986	17.130	1.00 23.23

ATOM	1423	CB	SER	Α	243	39.368	44.785	18.211	1.00 22.47
MOTA	1424	OG	SER	Α	243	38.515	44.386	19.274	1.00 23.32
ATOM	1425	N			244	37.635	42.115		
								16.979	1.00 20.52
ATOM	1426	CA			244	37.454	40.649	17.145	1.00 18.32
MOTA	1427	С	LEU	Α	244	37.535	39.844	15.860	1.00 18.66
ATOM	1428	0	LEU	Α	244	37.482	38.576	15.892	1.00 18.25
ATOM	1429	СВ	T.DII	7	244	36.120	40.368	17.843	1.00 18.01
MOTA	1430	CG			244	35.998	41.054	19.206	1.00 17.93
ATOM	1431		LEU			34.689	40.666	19.885	1.00 17.04
MOTA	1432	CD2	LEU	Α	244	37.189	40.661	20.063	1.00 19.23
ATOM	1433	N	TYR	Α	245	37.666	40.522	14.729	1.00 18.73
ATOM	1434	CA			245	37.756			
							39.795	13.459	1.00 19.72
MOTA	1435	С			245	38.536	40.545	12.398	1.00 20.55
MOTA	1436	0	TYR	Α	245	38.819	41.771	12.542	1.00 21.10
MOTA	1437	CB	TYR	Α	245	36.357	39.494	12.924	1.00 19.56
ATOM	1438	CG			245	35.606	40.708	12.421	1.00 20.40
ATOM	1439		TYR			34.977	41.586		
								13.302	1.00 20.11
ATOM	1440	CD2	TYR			35.512	40.966	11.055	1.00 20.70
MOTA	1441		TYR	Α	245	34.265	42.689	12.834	1.00 21.90
ATOM	1442	CE2	TYR	Α	245	34.809	42.060	10.573	1.00 22.10
MOTA	1443	CZ	TYR	Α	245	34.184	42.919	11.466	1.00 23.05
ATOM	1444	OH	TYR			33.476	43.993	10.979	1.00 22.53
ATOM	1445	N	THR			38.902	39.829	11.340	1.00 20.48
MOTA	1446	CA	THR	A	246	39.621	40.429	10.195	1.00 19.46
ATOM	1447	С	THR	Α	246	38.811	40.054	8.964	1.00 19.29
ATOM	1448	0	THR	Α	246	37.999	39.085	9.000	1.00 16.84
ATOM	1449		THR			41.049	39.865	10.031	1.00 19.69
ATOM									
	1450		THR			40.997	38.434	9.953	1.00 20.05
MOTA	1451	CG2	THR			41.929	40.294	11.194	1.00 19.01
MOTA	1452	N	GLY	Α	247	38.996	40.793	7.879	1.00 19.48
MOTA	1453	CA	GLY	Α	247	38.259	40.490	6.668	1.00 19.61
ATOM	1454	С			247	36.812	40.927	6.747	1.00 20.26
ATOM	1455								
		0	GLY			36.412	41.712	7.660	1.00 21.64
ATOM	1456	N	SER			36.006	40.437	5.816	1.00 21.23
MOTA	1457	CA	SER	Α	248	34.580	40.806	5.765	1.00 23.54
MOTA	1458	С	SER	Α	248	33.649	39.836	6.484	1.00 23.00
ATOM	1459	0	SER	Α	248	33.978	38.625	6.684	1.00 21.96
ATOM	1460	СВ	SER			34.135	40.936	4.304	1.00 24.06
ATOM	1461	OG	SER			34.814	41.999	3.656	1.00 28.27
MOTA	1462	N	LEU			32.494	40.355	6.881	1.00 23.33
MOTA	1463	CA	LEU	A	249	31.453	39.551	7.550	1.00 23.71
ATOM	1464	С	LEU	Α	249	30.478	39.103	6.468	1.00 23.26
ATOM	1465	0	LEU			29.913	39.958	5.721	1.00 24.66
ATOM	1466	СВ	LEU			30.687	40.392	8.576	
									1.00 22.83
MOTA	1467	CG	LEU			31.234	40.585	9.992	1.00 23.68
MOTA	1468		LEU			30.483	41.728	10.659	1.00 23.07
MOTA	1469	CD2	LEU	Α	249	31.077	39.299	10.802	1.00 22.16
MOTA	1470	N	TRP	Α	250	30.285	37.797	6.335	1.00 21.28
ATOM	1471	CA	TRP			29.328	37.282	5.348	1.00 18.03
MOTA	1472	C	TRP						
						28.115	36.810	6.115	1.00 18.51
MOTA	1473	0	TRP			28.242	36.079	7.153	1.00 18.65
MOTA	1474	CB	TRP	А	250	29.925	36.128	4.550	1.00 19.15
MOTA	1475	CG	TRP	Α	250	30.759	36.597	3.411	1.00 19.10
ATOM	1476		TRP			32.061	36.998	3.456	1.00 18.51
ATOM	1477		TRP						
						30.328	36.777	2.058	1.00 18.74
ATOM	1478		TRP			32.470	37.418	2.214	1.00 18.41
ATOM	1479		TRP			31.425	37.294	1.336	1.00 18.71
MOTA	1480	CE3	TRP	Α	250	29.118	36.554	1.386	1.00 19.61
ATOM	1481		TRP			31.352	37.594	-0.029	1.00 18.57
ATOM	1482		TRP					0.025	
						29.043	36.853		1.00 20.92
MOTA	1483		TRP			30.158	37.369	-0.666	1.00 17.98
MOTA	1484	N	TYR	A	251 ·	26.939	37.203	5.644	1.00 17.22

ATOM	1485	CA	TYR A	251	25.699	36.825	6.328	1.00 16.85
MOTA	1486	С	TYR A	251	24.875	35.751	5.642	1.00 16.82
ATOM	1487.	0	TYR A	251	24.668	35.782	4.397	1.00 17.05
ATOM	1488	СВ	TYR A		24.814	38.059	6.536	1.00 17.46
ATOM	1489	CG	TYR A					
					25.389	39.070	7.493	1.00 17.27
MOTA	1490	CD1	TYR A		26.265	40.065	7.055	1.00 18.34
MOTA	1491	CD2	TYR A	251	25.076	39.018	8.852	1.00 16.39
MOTA	1492	CE1	TYR A	251	26.819	40.984	7.955	1.00 18.20
ATOM	1493	CE2	TYR A	251	25.622	39.925	9.753	1.00 17.81
MOTA	1494	CZ	TYR A		26.487	40.900	9.302	1.00 17.43
ATOM	1495	OH	TYR A		27.014			•
						41.779	10.215	1.00 20.25
ATOM	1496	N	THR A		24.395	34.803	6.436	1.00 15.07
ATOM	1497	CA	THR A		23.525	33.725	5.933	1.00 14.48
MOTA	1498	С	THR A	252	22.204	33.996	6.646	1.00 16.15
ATOM	1499	0	THR A	252	22.193	34.429	7.845	1.00 16.66
ATOM	1500	CB	THR A	252	24.056	32.325	6.330	1.00 14.69
ATOM	1501	OG1	THR A	252	23.273	31.316	5.684	1.00 13.97
ATOM	1502	CG2	THR A		23.974	32.118	7.839	1.00 14.05
ATOM	1503	N	PRO A		21.070			
						33.774	5.972	1.00 15.93
ATOM	1504	CA	PRO A		19.826	34.054	6.694	1.00 17.09
ATOM	1505	С	PRO A		19.418	33.029	7.741	1.00 18.67
MOTA	1506	0	PRO A	253	19.782	31.813	7.653	1.00 17.11
MOTA	1507	CB	PRO A	253	18.789	34.161	5.572	1.00 17.20
ATOM	1508	CG	PRO A	253	19.304	33.207	4.545	1.00 17.18
ATOM	1509	CD	PRO A	253	20.809	33.468	4.553	1.00 17.14
ATOM	1510	N	ILE A		18.692	33.501	8.750	1.00 18.82
ATOM	1511	CA	ILE A		18.165			
						32.604	9.792	1.00 20.14
ATOM	1512	C	ILE A		16.885	32.091	9.137	1.00 21.33
MOTA	1513	0	ILE A		15.911	32.875	8.914	1.00 21.52
MOTA	1514	CB	ILE A	254	17.827	33.368	11.091	1.00 20.62
MOTA	1515	CG1	ILE A	254	19.124	33.752	11.806	1.00 20.82
MOTA	1516	CG2	ILE A	254	16.935	32.509	11.994	1.00 19.41
MOTA	1517	CD1	ILE A	254	18.920	34.458	13.127	1.00 22.19
ATOM	1518	N	ARG A		16.868	30.810	8.795	1.00 22.06
ATOM	1519	CA	ARG A		15.702	30.211	8.115	1.00 23.47
ATOM	1520	C	ARG A		14.398			
						30.343	8.880	1.00 24.68
ATOM	1521	0	ARG A		13.334	30.719	8.299	1.00 25.49
MOTA	1522	CB	ARG A		15.951	28.735	7.852	1.00 22.62
ATOM	1523	CG	ARG A		14.843	28.093	7.053	1.00 22.10
ATOM	1524	CD	ARG A	255	14.985	26.598	7.069	1.00 22.76
ATOM	1525	NE	ARG A	255	14.031	25.958	6.176	1.00 22.51
ATOM	1526	CZ	ARG A	255	13.692	24.679	6.256	1.00 22.37
ATOM	1527	NH1	ARG A	255	14.232	23.914	7.195	1.00 20.91
ATOM	1528		ARG A		12.819	24.166	5.396	1.00 23.78
ATOM	1529	N	ARG A		14.451	30.023	10.165	1.00 24.98
ATOM	1530							
		CA	ARG A		13.264	30.085	11.029	1.00 25.56
ATOM	1531	С	ARG A		13.723	30.441	12.438	1.00 24.84
ATOM	1532	0	ARG A		14.829	30.013	12.893	1.00 22.14
ATOM	1533	CB	ARG A	256	12.561	28.729	11.009	1.00 27.37
MOTA	1534	CG	ARG A	256	11.350	28.599	11.914	1.00 29.24
ATOM	1535	CD	ARG A	256	10.878	27.150	11.899	1.00 29.60
MOTA	1536	NE	ARG A		10.180	26.788	13.126	1.00 31.29
ATOM	1537	ČZ	ARG A		10.043	25.543	13.563	1.00 31.25
ATOM	1538		ARG A					1.00 31.19
ATOM	1539				10.559	24.535	12.870	
			ARG A		9.398	25.307	14.698	1.00 32.97
ATOM	1540	N	GLU A		12.914	31.219	13.141	1.00 24.01
ATOM	1541	CA	GLU A		13.270	31.650	14.500	1.00 23.46
MOTA	1542	C	GLU A	257	12.829	30.739	15.636	1.00 23.02
MOTA	1543	0	GLU A	257	11.749	30.947	16.264	1.00 26.15
MOTA	1544	CB	GLU A	257	12.739	33.055	14.748	1.00 23.25
ATOM	1545	CG	GLU A		13.439	34.123	13.930	1.00 26.24
ATOM	1546	CD	GLU A		12.572	35.353	13.746	1.00 27.27
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MOTA	1547	OET	GLU	Α	257		13.124	36.470	13.673	1.00 27.35
ATOM	1548	OE2	GLU	Α	257		11.334	35.197	13.665	1.00 30.46
ATOM	1549	N			258		13.632	29.719		
									15.898	1.00 19.64
MOTA	1550	CA			258		13.390	28.798	17.016	1.00 19.75
ATOM	1551	С	TRP	Α	258		14.812	28.548	17.495	1.00 19.46
ATOM	1552	0	TRP	Α	258		15.267	29.190	18.500	1.00 20.47
ATOM	1553	CB			258		12.632			
								27.537	16.561	1.00 18.27
MOTA	1554	CG			258		13.203	26.710	15.455	1.00 17.96
ATOM	1555	CD1	TRP	Α	258		13.898	27.143	14.364	1.00 18.43
ATOM	1556	CD2	TRP				13.051	25.293	15.298	
										1.00 17.87
ATOM	1557		TRP				14.187	26.082	13.537	1.00 18.62
MOTA	1558	CE2	TRP	Α	258		13.678	24.935	14.088	1.00 17.86
ATOM	1559.	CE3	TRP	Α	258		12.441	24.291	16.067	1.00 17.50
ATOM	1560	CZ2	TRP				13.717	23.614		
									13.624	1.00 19.19
ATOM	1561	CZ3	TRP				12.477	22.976	15.608	1.00 19.16
ATOM	1562	CH2	TRP	Α	258		13.113	22.650	14.396	1.00 18.86
ATOM	1563	N	TYR	Α	259		15.538	27.670	16.814	1.00 18.33
ATOM	1564	CA	TYR				16.965	27.458		
									17.126	1.00 15.42
ATOM	1565	С	TYR				17.550	28.474	16.157	1.00 16.46
ATOM	1566	0	TYR	Α	259		16.789	29.066	15.323	1.00 15.71
ATOM	1567	CB	TYR	Α	259		17.439	26.078	16.671	1.00 13.86
ATOM	1568	CG			259		17.056	24.927	17.564	
						•				1.00 13.98
ATOM	1569	CD1					17.876	24.539	18.627	1.00 13.32
MOTA	1570	CD2	TYR	Α	259		15.875	24.224	17.346	1.00 12.14
ATOM	1571	CE1	TYR	Α	259		17.520	23.467	19.450	1.00 15.06
MOTA	1572	CE2	TYR	Α	259		15.510	23.167	18.155	1.00 14.24
ATOM	1573	CZ	TYR				16.329	22.789		
									19.200	1.00 14.26
ATOM	1574	OH	TYR				15.940	21.719	19.955	1.00 12.92
MOTA	1575	N	TYR	A	260		18.851	28.725	16.224	1.00 14.50
ATOM	1576	CA	TYR	Α	260		19.440	29.630	15.232	1.00 15.21
ATOM	1577	С	TYR	Α	260		19.716	28.718	14.037	1.00 15.90
ATOM	1578	0	TYR				20.866	28.210	13.836	1.00 16.76
ATOM	1579	СВ	TYR				20.722	30.269	15.759	1.00 13.84
ATOM	1580	CG	TYR				20.426	31.416	16.690	1.00 14.32
MOTA	1581	CD1	TYR	Α	260		20.534	31.270	18.078	1.00 13.41
ATOM	1582	CD2	TYR	Α	260		19.996	32.642	16.187	1.00 13.45
ATOM	1583	CEI	TYR	Δ	260		20.224	32.320	18.933	1.00 13.15
ATOM	1584	CE2	TYR				19.680	33.699		
									17.037	1.00 12.56
MOTA	1585	CZ	TYR				19.801	33.530	18.404	1.00 13.22
MOTA	1586	OH	TYR	Α	260		19.531	34.582	19.239	1.00 12.88
MOTA	1587	N	GLU	Α	261		18.664	28.476	13.260	1.00 15.81
ATOM	1588	CA	GLU				18.741	27.586	12.081	1.00 17.54
ATOM	1589		GLU				19.191			
		С						28.266	10.791	1.00 17.31
ATOM	1590	0	GLU	A	261		18.665	29.355	10.402	1.00 16.63
MOTA	1591	CB	GLU	Α	261		17.382	26.914	11.842	1.00 16.53
ATOM	1592	CG	GLU	Α	261		17.326	26.076	10.573	1.00 19.47
MOTA	1593	CD	GLU				15.965	25.454	10.326	
ATOM	1594									1.00 20.18
			GLU				14.956	26.037	10.766	1.00 21.27
MOTA	1595	OE2	GLU				15.902	24.390	9.673	1.00 20.94
ATOM	1596	N	VAL	Α	262		20.153	27.640	10.122	1.00 16.45
ATOM	1597	CA	VAL	Α	262		20.679	28.147	8.842	1.00 16.13
ATOM	1598	С	VAL				20.620	27.006	7.831	1.00 17.33
ATOM	1599									
		σ	VAL				20.168	25.863	8.166	1.00 17.30
ATOM	1600	CB	VAL				22.131	28.624	8.982	1.00 14.58
MOTA	1601	CG1	VAL	Α	262		22.218	29.690	10.064	1.00 14.84
MOTA	1602		VAL				23.039	27.449	9.308	1.00 14.53
ATOM	1603	N	ILE				21.064	27.271	6.608	1.00 17.34
ATOM	1604	CA	ILE				21.044			
								26.245	5.554	1.00 16.67
MOTA	1605	C	ILE				22.419	26.042	4.931	1.00 16.64
MOTA	1606	0	ILE				23.054		4.418	1.00 17.50
ATOM	1607	CB	ILE	A	263		20.031	26.619	4.445	1.00 18.45
ATOM	1608	CG1	ILE	A	263		18.608	26.522	4.996	1.00 18.90

MOTA	1609	CG2	ILE A	263	20.192	25.694	3.243	1.00 18.17
MOTA	1610	CD1	ILE A	263	17.541	26.974	4.023	1.00 23.31
ATOM	1611.	N	ILE A		22.897	24.802	4.988	1.00 16.67
ATOM	1612	CA	ILE A					
					24.199	24.413	4.409	1.00 14.63
MOTA	1613	C	ILE A	•	23.882	23.836	3.031	1.00 16.44
ATOM	1614	0	ILE A		23.019	22.915	2.908	1.00 13.53
ATOM.	1615	CB	ILE A	264	24.877	23.320	5.253	1.00 14.79
ATOM	1616	CG1	ILE A	264	25.174	23.855	6.657	1.00 12.53
MOTA	1617	CG2	ILE A	264	26.154	22.846	4.563	1.00 12.07
ATOM	1618	CD1	ILE A		25.685	22.799	7.615	1.00 12.69
ATOM	1619	N						
			VAL A		24.546	24.334	1.992	1.00 17.37
MOTA	1620	CA	VAL A		24.258	23.841	0.627	1.00 18.64
MOTA	1621	C	VAL A		25.368	23.004	0.006	1.00 19.95
ATOM	1622	0	VAL A	265	25.202	22.455	-1.127	1.00 19.29
ATOM	1623	CB	VAL A	265	23.956	25.011	-0.322	1.00 18.56
ATOM	1624	CG1	VAL A	265	22.874	25.901	0.287	1.00 16.70
ATOM	1625	CG2	VAL A	265	25.227	25.802	-0.590	1.00 17.47
ATOM	1626	N	ARG A		26.486	22.872	0.707	1.00 20.42
ATOM	1627	CA	ARG A		27.617	22.098	0.165	
								1.00 20.48
ATOM	1628	C	ARG A		28.752	22.044	1.162	1.00 19.59
MOTA	1629	0	ARG A		29.030	23.055	1.885	1.00 19.51
MOTA	1630	CB	ARG A	266	28.112	22.763	-1.129	1.00 22.33
ATOM	1631	CG	ARG A	266	29.417	22.218	-1.713	1.00 22.40
MOTA	1632	CD	ARG A	266	29.939	23.170	-2.789	1.00 24.49
ATOM	1633	NE	ARG A		31.244	22.785	-3.322	1.00 24.49
ATOM	1634	CZ	ARG A		31.444	22.266	-4.528	1.00 26.46
ATOM	1635	NH1			30.426	22.061	-5.349	1.00 25.31
MOTA	1636	NH2						
					32.672	21.956	-4.920	1.00 27.88
MOTA	1637	N	VAL A		29.404	20.891	1.246	1.00 18.31
ATOM	1638	CA	VAL A		30.561	20.766	2.136	1.00 18.32
MOTA	1639	С	VAL A	267	31.671	20.072	1.369	1.00 18.25
ATOM	1640	0	VAL A	267	31.409	19.192	0.489	1.00 19.14
MOTA	1641	CB	VAL A	267	30.248	19.974	3.456	1.00 18.72
ATOM	1642	CG1	VAL A	267	28.784	19.645	3.547	1.00 18.30
ATOM	1643		VAL A		31.112	18.728	3.554	1.00 17.65
ATOM	1644	N	GLU A		32.903	20.471	1.647	1.00 16.18
MOTA	1645	CA	GLU A		34.046	19.848	0.990	1.00 17.71
ATOM	1646	C	GLU A		35.169	19.546	1.970	1.00 16.08
ATOM	1647	0	GLU A		35.293	20.191	3.064	1.00 13.62
ATOM	1648	CB	GLU A		34.550	20.717	-0.177	1.00 18.50
ATOM	1649	CG	GLU A		34.430	22.207	0.030	1.00 22.46
MOTA	1650	CD	GLU A	268	34.888	23.016	-1.181	1.00 22.13
ATOM	1651	OE1	GLU A	268	34.216	22.970	-2.237	1.00 20.91
ATOM	1652		GLU A		35.927	23.703	-1.067	1.00 22.44
MOTA	1653	N	ILE A		35.948	18.531	1.623	1.00 13.57
ATOM	1654	CA	ILE A		37.103	18.112	2.418	1.00 13.89
ATOM	1655	C	ILE A		38.259	18.448	1.485	1.00 14.06
ATOM								
	1656	0	ILE A		38.396	17.832	0.386	1.00 14.03
MOTA	1657	CB	ILE A		37.051	16.596	2.703	1.00 14.48
MOTA	1658		ILE A		35.697	16.239	3.327	1.00 14.59
MOTA	1659	CG2			38.180	16.193	3.645	1.00 12.12
MOTA	1660	CD1	ILE A	269	35.358	17.022	4.592	1.00 13.16
MOTA	1661	N	ASN A	270	39.067	19.431	1.872	1.00 14.16
ATOM	1662	CA	ASN A		40.205	19.886	1.038	1.00 13.20
MOTA	1663	C	ASN A		39.774	20.177	-0.399	1.00 13.24
ATOM	1664	ō	ASN A		40.427	19.714	-1.385	1.00 13.72
MOTA	1665	СВ	ASN A		41.336			1.00 13.72
						18.852	1.047	
MOTA	1666	CG	ASN A		42.424	19.186	2.054	1.00 13.23
ATOM	1667		ASN A		42.339	20.224	2.790	1.00 13.62
MOTA	1668		ASN A		43.454	18.348	2.117	1.00 11.67
MOTA	1669	N	GLY A		38.691	20.932	-0.540	1.00 13.07
MOTA	1670	CA	GLY A	271	38.210	21.302	-1.858	1.00 13.58
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ATOM	1671	С	GLY A 27			-2.564	1.00	14.87
ATOM	1672	0	GLY A 27		20.545	-3.581	1.00	13.70
ATOM	1673		GLN A 27		19.005	-2.076	1.00	14.64
ATOM	1674	CA	GLN A 27			-2.705	1.00	14.45
ATOM	1675	C	GLN A 27		17.870	-2.140	1.00	15.83
ATOM	1676	0	GLN A 27		17.717	-0.902		15.81
ATOM	1677	CB	GLN A 27		16.561	-2.486		14.85
MOTA	1678	CG	GLN A 27:		15.421	-3.250		14.45
MOTA	1679	CD	GLN A 27		14.135	-3.211		16.34
ATOM	1680		L GLN A 272		13.134	-2.535	1.00	20.05
ATOM	1681		2 GLN A 272		14.121	-3.909	1.00	13.09
ATOM	1682	N	ASP A 273		17.995	-3.035	1.00	16.17
ATOM	1683	CA	ASP A 273		17.987	-2.686	1.00	17.89
ATOM	1684	С	ASP A 273		16.612	-2.201	1.00	16.92
ATOM	1685	0	ASP A 273		15.566	-2.831	1.00	16.53
ATOM	1686	CB	ASP A 273		18.395	-3.930	1.00	20.38
MOTA	1687	CG	ASP A 273		18.526	-3.665	1.00	20.89
ATOM	1688		ASP A 273		18.788	-4.630	1.00	21.98
ATOM	1689		ASP A 273		18.378	-2.503		22.40
ATOM	1690	N	LEU A 274		16.576	-1.101 ⁻	1.00	
ATOM	1691	CA	LEU A 274		15.285	-0.587	1.00	
ATOM	1692	C	LEU A 274		14.805	-1.598	1.00	
ATOM	1693	0	LEU A 274		13.603	-1.623	1.00	
ATOM	1694	CB	LEU A 274		15.455	0.783	1.00	
MOTA	1695	CG	LEU A 274		15.595	2.011	1.00	
MOTA	1696		LEU A 274		15.558	3.267	1.00	
ATOM	1697		LEU A 274		14.463	2.050	1.00	
ATOM ATOM	1698 1699	N	LYS A 275		15.736	-2.431	1.00	
ATOM	1700	CA C	LYS A 275		15.452	-3.501	1.00	
ATOM	1701	0	LYS A 275		14.715	-3.000	1.00	
ATOM	1701	СВ	LYS A 275		13.586	-3.464	1.00	
ATOM	1702	CG	LYS A 275		14.642	-4.608	1.00	
ATOM	1704	CD	LYS A 275		14.818	-5.970	1.00	
ATOM	1705	CE.	LYS A 275		14.059	-7.042	1.00	
ATOM	1706	NZ	LYS A 275		14.297 15.759	-8.408	1.00	
ATOM	1707	N	MET A 276		15.739	-8.702	1.00	
ATOM	1708	CA	MET A 276		14.722	-2.063 -1.505	1.00	
ATOM	1709	C	MET A 276		15.592	-1.815	1.00	
ATOM	1710	Ō	MET A 276		16.818	-2.117	1.00	
ATOM	1711	СВ	MET A 276		14.576	0.011	1.00	
ATOM	1712	CG	MET A 276		13.605	0.469	1.00	
MOTA	1713	SD	MET A 276	26.687	13.418	2.261	1.00	
MOTA	1714	CE	MET A 276		12.457	2.477	1.00	
MOTA	1715	N	ASP A 277	23.136	14.994	-1.756	1.00	
ATOM	1716	CA	ASP A 277	21.906	15.750	-1.994	1.00	
MOTA	1717	C	ASP A 277	21.903	16.864	-0.955	1.00 3	
ATOM	1718	0	ASP A 277	22.070	16.608	0.278	1.00 3	
MOTA	1719	CB	ASP A 277	20.682	14.851	-1.818	1.00 3	
ATOM	1720	CG	ASP A 277	19.377	15.595	-2.029	1.00 3	
MOTA	1721	OD1	ASP A 277	18.332	14.925	-2.168	1.00 4	
MOTA	1722	OD2	ASP A 277	19.386	16.844	-2.049	1.00 3	
MOTA	1723	N	CYS A 278	21.732	18.089	-1.432	1.00 3	34.50
ATOM	1724	CA	CYS A 278	21.725	19.294	-0.581	1.00 3	
ATOM	1725	С	CYS A 278	20.988	19.126	0.749	1.00 3	
ATOM	1726	0	CYS A 278	21.503	19.540	1.834	1.00 3	34.38
ATOM	1727	СВ	CYS A 278	21.108	20.460	-1.362	1.00 3	39.86
ATOM	1728	SG	CYS A 278	21.760	22.075	-0.852	1.00 5	
MOTA	1729	N	LYS A 279	19.802	18.529	0.705	1.00 3	
ATOM	1730	CA	LYS A 279	19.003	18.359	1.931	1.00 3	
ATOM	1731	C	LYS A 279	19.584	17.430	2.996	1.00 3	
MOTA	1732	0	LYS A 279	19.173	17.501	4.189	1.00 2	7.89

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MOTA	1733	CB	LYS			17.574	17.939	1.567	1.00 34.74
MOTA	1734	CG	LYS	Α	279	17.459	16.765	0.612	1.00 39.08
MOTA	1735	CD	LYS	Α	279	17.576	15.429	1.326	1.00 41.32
ATOM	1736	CE	LYS			17.185	14.289	0.393	1.00 42.86
ATOM	1737	NZ	LYS			17.118	12.978	1.099	1.00 45.07
MOTA	1738	N	GLU	Α	280	20.525	16.570	2.621	1.00 27.06
MOTA	1739	CA	GLU	Α	280	21.141	15.659	3.612	1.00 26.22
MOTA	1740	С	GLU	Α	280	21.900	16.458	4.673	1.00 25.34
ATOM	1741	0	GLU			21.920	16.074	5.886	1.00 23.01
ATOM	1742	CB	GLU			22.109	14.693	2.928	1.00 27.98
MOTA	1743	CG	GLU	Α	280	21.459	13.725	1.946	1.00 31.24
ATOM	1744	CD	GLU	Α	280	20.486	12.765	2.610	1.00 32.55
ATOM	1745	OE1	GLU	Α	280	20.447	12.704	3.857	1.00 33.21
ATOM	1746		GLU			19.763	12.058	1.878	1.00 34.72
ATOM	1747	N	TYR			22.515	17.562	4.255	1.00 23.32
MOTA	1748	CA	TYR	Α	281	23.295	18.420	5.176	1.00 22.69
MOTA	1749	С	TYR	Α	281	22.415	19.082	6.219	1.00 23.40
ATOM	1750	0	TYR	Α	281	22.904	19.470	7.327	1.00 23.11
ATOM	1751	CB			281	24.035	19.515	4.400	1.00 20.26
			TYR						
MOTA	1752	CG				24.958	18.993	3.328	1.00 19.39
MOTA	1753		TYR			25.858	17.961	3.601	1.00 17.78
MOTA	1754	CD2	TYR	Α	281	24.943	19.534	2.042	1.00 18.55
MOTA	17 55	CE1	TYR	Α	281	26.719	17.478	2.623	1.00 17.05
ATOM	1756	CE2	TYR	Α	281	25.808	19.058	1.051	1.00 18.53
ATOM	1757	CZ			281	26.692	18.028	1.355	1.00 17.87
MOTA	1758	OH	TYR			27.558	17.533	0.407	1.00 18.13
MOTA	1759	N	ASN	Α	282	21.136	19.232	5.899	1.00 22.82
ATOM	1760	CA	ASN	Α	282	20.194	19.881	6.820	1.00 23.17
MOTA	1761	C	ASN	Α	282	19.089	18.922	7.238	1.00 23.84
ATOM	1762	ō			282	17.987	19.366	7.685	1.00 21.83
ATOM	1763	CB			282	19.598	21.111	6.137	1.00 22.42
MOTA	1764	CG	ASN	Α	282	20.665	22.018	5.549	1.00 23.90
MOTA	1765	OD1	ASN	Α	282	21.426	22.693	6.298	1.00 23.87
MOTA	1766	ND2	ASN	A	282	20.760	22.044	4.224	1.00 23.36
ATOM	1767	N			283	19.343	17.623	7.102	1.00 25.74
ATOM	1768	CA			283	18.322	16.633	7.472	1.00 28.01
MOTA	1769	C			283	17.905	16.843	8.912	1.00 29.29
ATOM	1770	0			283	18.686	16.572	9.881	1.00 27.50
MOTA	1771	CB	TYR	Α	283	18.810	15.200	7.280	1.00 29.52
MOTA	1772	CG	TYR	Α	283	17.783	14.200	7.756	1.00 31.64
ATOM	1773	CD1	TYR	Α	283	16.428	14.374	7.460	1.00 32.38
ATOM	1774		TYR			18.153	13.098	8.523	1.00 33.44
ATOM									
	1775		TYR			15.468	13.479	7.919	1.00 33.96
MOTA	1776		TYR			17.201	12.194	8.987	1.00 35.48
MOTA	1777	CZ			283	15.860	12.392	8.683	1.00 35.35
ATOM	1778	OH	TYR	Α	283	14.918	11.504	9.149	1.00 36.54
ATOM	1779	N	ASP	Α	284	16.665	17.299	9.043	1.00 30.23
ATOM	1780	CA			284	16.026	17.638	10.312	1.00 28.41
ATOM	1781	C			284	16.273	19.129	10.409	1.00 27.12
MOTA	1782	0			284	15.309	19.953	10.305	1.00 25.19
MOTA	1783	CB			284	16.684	16.928	11.494	1.00 33.07
MOTA	1784	CG	ASP	A	284	16.035	17.283	12.813	1.00 33.49
ATOM	1785	DD1	ASP	Α	284	16.520	16.815	13.860	1.00 37.38
ATOM	1786		ASP			15.035	18.031	12.802	1.00 35.95
ATOM	1787	N					19.499	10.563	1.00 22.62
					285	17.542			
ATOM	1788	CA			285	17.914	20.927	10.678	1.00 20.42
MOTA	1789	С			285	19.420	21.145	10.812	1.00 19.89
MOTA	1790	0	LYS	Α	285	20.209	20.174	11.037	1.00 19.63
ATOM	1791	CB	LYS	Α	285	17.230	21.540	11.903	1.00 18.63
ATOM	1792	CG			285	17.753	20.987	13.232	1.00 16.63
ATOM	1793	CD			285	16.966	21.538	14.421	1.00 14.93
		CE			285		21.088	15.754	1.00 15.57
MOTA	1794	CE	பரவ	A	203	17.551	21.000	10.104	2.00 13.37

ATOM	1795	NZ	LYS A	285	17.482	19.606	15.974	1.00 13.50
ATOM	1796	N	SER A	286	19.827	22.402	10.678	1.00 17.19
ATOM	1797	CA	SER A		21.241	22.808	10.827	1.00 16.52
ATOM	1798	C	SER A					
					21.228	24.034	11.727	1.00 15.74
MOTA	1799	0	SER A		20.592	25.080	11.377	1.00 14.46
MOTA	1800	CB	SER A	286	21.862	23.179	9.475	1.00 16.90
ATOM	1801	OG	SER A	286	22.064	22.036	8.671	1.00 16.60
ATOM	1802	N	ILE A		21.900	23.946	12.870	1.00 13.25
	1803	CA						
ATOM			ILE A		21.933	25.079	13.805	1.00 13.97
MOTA	1804	С	ILE A	287	23.342	25.511	14.206	1.00 15.14
MOTA	1805	0	ILE A	287	24.346	24.750	14.024	1.00 14.63
ATOM	1806	CB	ILE A	287	21.145	24.757	15.102	1.00 13.55
ATOM	1807	CG1			21.898	23.717	15.929	1.00 12.52
ATOM	1808	CG2			19.758			
						24.214	14.754	1.00 12.10
ATOM	1809	CD1			21.274	23.455	17.283	1.00 14.43
ATOM	1810	N	VAL A	288	23.431	26.728	14.732	1.00 14.78
ATOM	1811	CA	VAL A	288	24.701	27.292	15.223	1.00 15.54
ATOM	1812	С	VAL A	288	24.510	27.262	16.733	1.00 16.05
ATOM	1813	0.	VAL A		23.571	27.930	17.278	1.00 15.61
ATOM	1814	•	VAL A					
		CB			24.896	28.751	14.767	1.00 15.19
MOTA	1815		VAL A		26.248	29.259	15.239	1.00 14.78
ATOM	1816	CG2	VAL A	288	24.791	28.842	13.246	1.00 15.19
ATOM	1817	N	ASP A	289	25.355	26.512	17.430	1.00 15.91
ATOM	1818	CA	ASP A	289	25.194	26.373	18.891	1.00 14.81
ATOM	1819	C	ASP A		26.467	26.444	19.724	1.00 15.27
ATOM								
	1820	0	ASP A		27.322	25.504	19.700	1.00 15.75
MOTA	1821	CB	ASP A		24.467	25.060	19.168	1.00 12.65
ATOM	1822	CG	ASP A	289	24.264	24.806	20.634	1.00 13.29
ATOM	1823	OD1	ASP A	289	24.372	25.768	21.426	1.00 11.88
ATOM	1824		ASP A		23.981	23.639	20.988	1.00 10.63
ATOM	1825	N	SER A		26.604			
						27.529	20.479	1.00 15.19
MOTA	1826	CA	SER A		27.782	27.730	21.346	1.00 14.55
MOTA	1827	С	SER A	290	27.770	26.748	22.510	1.00 15.43
ATOM	1828	0	SER A	290	28.823	26.539	23.186	1.00 13.77
ATOM	1829	CB	SER A	290	27.795	29.165	21.888	1.00 15.33
ATOM	1830	OG	SER A		26.614	29.442	22.620	1.00 12.79
ATOM	1831	N	GLY A		26.612	26.137	22.759	1.00 14.34
ATOM	1832	CA	GLY A					
					26.486	25.192	23.856	1.00 14.93
ATOM	1833	С	GLY A		26.779	23.751	23.479	1.00 16.64
ATOM	1834	0	GLY A		26.502	22.792	24.277	1.00 14.49
ATOM	1835	N	THR A	292	27.305	23.556	22.277	1.00 16.47
ATOM	1836	CA	THR A	292	27.674	22.202	21.812	1.00 15.30
MOTA	1837	С	THR A	292	29.159	22.215	21.482	1.00 14.67
ATOM	1838	0	THR A		29.653	23.102	20.725	1.00 13.26
MOTA	1839	CB	THR A		26.889	21.784	20.550	1.00 15.29
ATOM	1840		THR A		25.522	21.521	20.895	1.00 13.88
ATOM	1841	CG2	THR A	292	27.514	20.527	19.932	1.00 13.59
MOTA	1842	N	THR A	293	29.887	21.253	22.027	1.00 14.43
ATOM	1843	CA	THR A	293	31.343	21.162	21.801	1.00 12.76
ATOM	1844	С	THR A		31.749	20.906	20.348	1.00 14.47
ATOM	1845	0	THR A		32.478	21.735	19.712	1.00 14.61
ATOM	1846	CB	THR A		31.949	20.035	22.650	1.00 12.36
MOTA	1847		THR A		31.726	20.304	24.041	1.00 10.79
MOTA	1848	CG2	THR A	293	33.437	19.916	22.382	1.00 9.56
MOTA	1849	N	ASN A	294	31.286	19.783	19.810	1.00 13.53
MOTA	1850	CA	ASN A		31.648	19.349	18.440	1.00 15.26
ATOM	1851	C	ASN A		30.871	19.917	17.276	1.00 15.45
ATOM	1852	0	ASN A		29.851	20.662	17.431	1.00 13.68
ATOM	1853	CB	ASN A		31.494	17.832	18.307	1.00 14.81
MOTA	1854	CG	ASN A		32.351	17.051	19.270	1.00 14.13
MOTA	1855	OD1	ASN A	294	32.264	15.791	19.304	1.00 19.85
ATOM	1856	ND2	ASN A	294	33.174	17.734	20.051	1.00 13.25

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ATOM	1857	N			295	31.365	19.556	16.096	1.00 15.21
MOTA	1858	CA	LEU	Α	295	30.689	19.866	14.835	1.00 15.29
ATOM	1859.	С	LEU	Α	295	29.924	18.548	14.719	1.00 16.43
ATOM	1860	0	LEU			30.556	17.452		
ATOM	1861	СВ						14.575	1.00 16.34
			LEU			31.674	19.963	13.671	1.00 13.54
MOTA	1862	CG.	LEU			31.017	19.837	12.287	1.00 14.74
MOTA	1863	CD1	LEU	Α	295	29.991	20.947	12.109	1.00 14.37
ATOM	1864	CD2	LEU	A	295	32.073	19.903	11.179	1.00 13.91
ATOM	1865	Ŋ			296	28.606	18.591	14.831	1.00 16.08
ATOM	1866	CA			296				
						27.827	17.349	14.719	1.00 17.47
ATOM	1867	C			296	27.180	17.300	13.343	1.00 17.04
MOTA	1868	0	ARG	A	296	26.655	18.339	12.840	1.00 15.28
ATOM.	1869 .	CB	ARG	Α	296	26.785	17.290	15.834	1.00 18.37
MOTA	1870	CG	ARG	Α	296	27.421		17.208	1.00 19.73
MOTA	1871	CD			296	26.425	17.262	18.324	1.00 22.63
ATOM	1872	NE	ARG						
						26.292	15.867	18.722	1.00 25.23
MOTA	1873	CZ			296	25.135	15.223	18.776	1.00 26.52
ATOM	1874		ARG			24.011	15.851	18.446	1.00 27.11
ATOM	1875	NH2	ARG	Α	296	25.100	13.961	19.179	1.00 27.00
ATOM	1876	N .	LEU	Α	297	27.211	16.123	12.722	1.00 15.65
ATOM	1877	CA	LEU			26.660	15.945	11.356	1.00 15.33
ATOM	1878	C	LEU			25.657	14.800	11.246	
ATOM	1879								1.00 17.46
		0 .	LEU			25.795	13.743	11.938	1.00 16.37
MOTA	1880	CB	LEU			27.806	15.681	10.371	1.00 12.00
ATOM	1881	CG	LEU	Α	297	28.925	16.729	10.277	1.00 11.84
MOTA	1882	CD1	LEU	A	297	30.136	16.148	9.561	1.00 8.16
MOTA	1883	CD2	LEU	Α	297	28.410	17.962	9.559	1.00 8.99
ATOM	1884	N			298	24.636	14.960	10.386	1.00 19.11
ATOM	1885	CA			298				
						23.636	13.901	10.217	1.00 20.53
ATOM	1886	C			298	24.387	12.619	9.868	1.00 21.03
ATOM	1887	0	PRO	Α	298	25.419	12.668	9.131	1.00 21.77
MOTA	1888	CB	PRO	Α	298	22.788	14.411	9.054	1.00 19.18
MOTA	1889	CG	PRO	Α	298	22.861	15.897	9.209	1.00 20.46
ATOM	1890	CD	PRO	Α	298	24.335	16.111	9.517	1.00 19.69
ATOM	1891	N	LYS			23.911	11.487	10.376	1.00 22.77
ATOM	1892	CA	LYS			24.562	10.169	10.137	
ATOM	1893	C	LYS						1.00 25.34
						25.169	9.979	8.753	1.00 24.56
ATOM	1894	0	LYS		•	26.393	9.681	8.617	1.00 22.24
ATOM	1895	CB	LYS			23.566	9.034	10.387	1.00 29.05
MOTA	1896	CG	LYS	Α	299	24.156	7.650	10.146	1.00 33.27
MOTA	1897	CD	LYS	Α	299	23.144	6.547	10.408	1.00 37.10
MOTA	1898	CE	LYS	Α	299	23.758	5.178	10.151	1.00 38.78
MOTA	1899	NZ	LYS	Α	299	22.775	4.077	10.380	1.00 42.51
ATOM	1900	N	LYS			24.340	10.127	7.729	1.00 24.24
ATOM	1901	CA	LYS						
						24.774	9.955	6.333	1.00 25.41
MOTA	1902	C	LYS			25.901	10.916	5.952	1.00 24.12
MOTA	1903	0	LYS			26.889	10.515	5.262	1.00 23.67
MOTA	1904	CB	LYS	Α	300	23.576	10.154	5.403	1.00 28,77
ATOM	1905	CG	LYS	Α	300	23.788	9.660	3.990	1.00 33.37
MOTA	1906	CD	LYS	A	300	22.661	8.718	3.569	1.00 38.01
MOTA	1907	CE	LYS			21.298	9.393	3.652	1.00 40.18
ATOM	1908	NZ	LYS						
ATOM						20.191	8.455	3.291	1.00 42.69
	1909	N	VAL			25.784	12.172	6.368	1.00 20.46
ATOM	1910	CA	VAL		=	26.832	13.169	6.058	1.00 18.21
MOTA	1911	С	VAL			28.083	12.842	6.867	1.00 17.93
MOTA	1912	0	VAL	A	301	29.241	12.929	6.343	1.00 16.84
MOTA	1913	CB	VAL	Α	301	26.358	14.601	6.391	1.00 17.29
MOTA	1914		VAL			27.468	15.605	6.105	1.00 15.43
ATOM	1915		VAL			25.118	14.935	5.565	1.00 16.34
ATOM	1916	N	PHE			27.887			
							12.448	8.122	1.00 17.43
ATOM	1917	CA	PHE			29.032	12.099	8.990	1.00 18.16
MOTA	1918	С	PHE	A	302	29.854	10.957	8.399	1.00 18.95

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MOTA	1919	0	PHE			31.121	11.004	8.399	1.00 18.60
ATOM	1920	CB	PHE	Α	302	28.550	11.713	10.391	1.00 17.38
MOTA	1921 -	CG	PHE	A	302	29.639	11.180	11.265	1.00 19.16
	1922		PHE				9.810		
ATOM						29.866		11.362	1.00 17.81
MOTA	1923	CD2	PHE	Α	302	30.498	12.051	11.923	1.00 18.89
ATOM	1924	CE1	PHE	Α	302	30.934	9.320	12.096	1.00 19.63
ATOM	1925		PHE			31.573	11.569	12.660	1.00 19.90
MOTA	1926	CZ	PHE			31.793	10.201	12.747	1.00 19.13
ATOM	1927	N	GLU	Α	303	29.172	9.931	7.901	1.00 19.20
ATOM	1928	CA	GLU	Α	303	29.859	8.769	7.295	1.00 21.56
	1929	C				30.679	9.189	6.083	
ATOM			GLU						1.00 19.19
MOTA	1930	0	GLU	Α	303	31.865	8.777	5.929	1.00 18.04
ATOM	1931	CB	GLU	Α	303	28.836	7.704	6.888	1.00 24.72
ATOM	1932	CG	GLU	Α	303	28.246	6.939	8.069	1.00 29.90
ATOM	1933	CD	GLU			27.051	6.076	7.683	1.00 33.77
ATOM	1934	OE1	GLU	Α	303	26.585	5.294	8.541	1.00 36.31
ATOM	1935	OE2	GLU	Α	303	26.572	6.183	6.528	1.00 36.51
ATOM	1936	N	ALA	А	304	30.088	9.998	5.216	1.00 17.86
	1937	CA				30.805			1.00 18.11
MOTA			ALA				10.472	4.007	
MOTA	1938	С	ALA	Α	304	31.999	11.354	4.386	1.00 17.49
ATOM	1939	0	ALA	Α	304	33.102	11.242	3.777	1.00 17.76
ATOM	1940	CB	ALA	Α	304	29.849	11.244	3.102	1.00 17.14
ATOM	1941	N	ALA			31.812	12.221	5.377	1.00 17.06
MOTA	1942	CA	ALA			32.900	13.128	5.829	1.00 16.43
ATOM	1943	C	ALA	Α	305	34.092	12.387	6.440	1.00 16.39
MOTA	1944	0	ALA	Α	305	35.272	12.644	6.054	1.00 17.78
ATOM	1945 4	CB	ALA	Α	305	32.351	14.140	6.833	1.00 15.92
ATOM	1946	N	VAL			33.842	11.476	7.375	1.00 15.50
MOTA	1947	CA	VAL			34.971	10.756	8.004	1.00 17.31
MOTA	1948	С	VAL	Α	306	35.719	9.920	6.987	1.00 16.95
MOTA	1949	0	VAL	Α	306	36.983	9.829	7.029	1.00 16.21
ATOM	1950	CB	VAL	Α	306	34.514	9.845	9.162	1.00 17.93
ATOM	1951		VAL			33.954	10.693	10.280	1.00 19.37
ATOM	1952		VAL			33.477	8.851	8.669	1.00 19.63
ATOM	1953	N	LYS	A	307	34.987	9.307	6.065	1.00 17.11
ATOM	1954	CA	LYS	A	307	35.641	8.488	5.032	1.00 18.39
ATOM	1955	С	LYS	Α	307	36.654	9.350	4.279	1.00 17.59
ATOM	1956	ō	LYS			37.848	8.959	4.107	1.00 18.09
					•				
ATOM	1957	СВ	LYS			34.602	7.940	4.052	1.00 19.72
ATOM	1958	CG	LYS	Α	307	35.212	7.112	2.930	1.00 24.02
ATOM	1959	CD	LYS	Α	307	34.147	6.415	2.102	1.00 26.72
ATOM	1960	CE	LYS	Α	307	34.779	5.505	1.058	1.00 29.36
	1961	NZ	LYS			33.745	4.869		1.00 31.68
MOTA									
ATOM	1962	N			308	36.205	10.520	3.842	1.00 16.75
MOTA	1963	CA	SER	A	308	37.059	11.460	3.091	1.00 17.46
MOTA	1964	C	SER	Α	308	38.198	12.000	3.953	1.00 16.11
ATOM	1965	0			308	39.378	12.056	3.501	1.00 17.12
ATOM	1966	СB			308			2.560	1.00 17.51
						36.208	12.620		
MOTA	1967	OG			308	36.982	13.505	1.774	1.00 19.76
MOTA	1968	И	ILE	Α	309	37.886	12.400	5.180	1.00 16.07
ATOM	1969	CA	ILE	A	309	38.926	12.927	6.083	1.00 14.41
MOTA	1970	C			309	39.945	11.831	6.378	1.00 14.93
		•							1.00 14.90
MOTA	1971	0			309	41.171	12.112	6.505	
MOTA	1972	CB			309	38.310	13.439	7.401	1.00 13.88
MOTA	1973	CG1	ILE	Α	309	37.346	14.595	7.099	1.00 13.08
ATOM	1974		ILE			39.404	13.887	8.350	1.00 11.40
ATOM	1975		ILE			36.575	15.084	8.315	1.00 12.70
	1976	N							1.00 15.62
MOTA					310	39.475	10.592	6.485	
MOTA	1977	CA			310	40.375	9.437	6.752	1.00 17.74
ATOM	1978	C	LYS	Α	310	41.289	9.223	5.559	1.00 17.22
ATOM	1979	0	LYS	Α	310	42.532	9.061	5.715	1.00 16.87
ATOM	1980	CB			310	39.577	8.149	6.976	1.00 18.35
						,			

MOTA	1981	CG		A 310	39.003	7.953	8.373	1.00 20.85
MOTA	1982	CD	LYS A	A 310	38.269	6.617	8.432	1.00 22.02
MOTA	1983	CE	LYS Z	A 310	37.584	6.404	9.757	1.00 25.26
MOTA	1984	NZ	T.VC	A 310	36.808	5.129	9.752	1.00 26.15
ATOM	1985	N		A 311	40.698	9.211		
							4.370	1.00 15.56
ATOM	1986	CA		A 311	41.466	9.007	3.124	1.00 17.77
MOTA	1987	С	ALA A	A 311	42.549	10.071	2.990	1.00 17.36
ATOM	1988	0	ALA Z	A 311	43.708	9.768	2.578	1.00 20.71
ATOM	1989	СВ		A 311	40.524	9.047	1.908	1.00 14.11
MOTA	1990	N		A 312	42.210	11.309		
							3.330	1.00 16.63
MOTA	1991	CA		A 312	43.184	12.418	3.235	1.00 15.73
MOTA	1992	C	ALA A	A 312	44.247	12.342	4.333	1.00 15.59
MOTA	1993	0	ALA A	A 312	45.348	12.958	4.207	1.00 13.09
ATOM	1994	CB	ALA Z	A 312	42.449	13.758	3.301	1.00 13.50
ATOM	1995	N		A 313	43.950	11.593	5.393	1.00 17.05
MOTA	1996	CA		A 313	44.867	11.432		
							6.560	1.00 19.05
ATOM	1997	C		A 313	45.579	10.085	6.593	1.00 19.49
MOTA	1998	0	SER A	A 313	46.332	9.787	7.568	1.00 21.95
MOTA	1999	CB	SER I	A 313	44.075	11.555	7.865	1.00 17.23
ATOM	2000	OG	SER I	A 313	43.501	12.834	8.003	1.00 23.58
ATOM	2001	N	SER 2	A 314	45.368	9.270	5.570	1.00 20.76
ATOM	2002	CA		A 314	45.952	7.909	5.513	1.00 22.73
	2002							
ATOM		C		A 314	47.436	7.725	5.838	1.00 21.90
MOTA	2004	0		A 314	47.825	6.639	6.359	1.00 20.76
ATOM	2005	CB	SER I	A 314	45.650	7.271	4.150	1.00 22.50
ATOM	2006	OG	SER I	A 314	46.207	8.032	3.093	1.00 27.94
ATOM	2007	N	THR I	A 315	48.285	8.714	5.570	1.00 20.90
ATOM	2008	CA	THR	A 315	49.732	8.523	5.868	1.00 23.78
ATOM	2009	C		A 315	50.020	8.454	7.361	1.00 25.42
	2010							
ATOM		0		A 315	51.191	8.219	7.784	1.00 26.24
MOTA	2011	СВ		A 315	50.616	9.634	5.257	1.00 23.59
MOTA	2012			A 315	50.256	10.901	5.818	1.00 22.73
ATOM	2013	CG2		A 315	50.456	9.668	3.745	1.00 22.59
MOTA	2014	N	GLU 2	A 316	48.994	8.655	8.176	1.00 27.46
ATOM	2015	CA	GLU .	A 316	49.170	8.589	9.638	1.00 29.81
ATOM	2016	С		A 316	48.258	7.503	10.201	1.00 30.55
ATOM	2017	0.		A 316	47.110	7.314	9.710	1.00 29.51
ATOM	2018	СВ		A 316	48.819	9.931	10.279	1.00 23.51
ATOM	2019	CG		A 316	49.277	10.039	11.725	1.00 36.72
ATOM	2020	CD		A 316	50.571	10.818	11.879	1.00 36.99
MOTA	2021	OE1		A 316	51.456	10.728	11.003	1.00 37.39
MOTA	2022	OE2	GLU .	A 316	50.704	11.522	12.893	1.00 41.14
MOTA	2023	N	LYS :	A 317	48.736	6.775	11.205	1.00 32.69
ATOM	2024	CA		A 317	47.928	5.702	11.828	1.00 35.09
	2025	C		A 317	47.216	6.223	13.071	1.00 33.44
MOTA	2026	Õ		A 317	47.804	7.005	13.883	1.00 34.13
MOTA	2027	CB		A 317	48.809	4.505	12.202	1.00 38.52
MOTA	2028	CG		A 317	49.980	4.844	13.106	1.00 43.41
MOTA	2029	CD	LYS .	A 317	50.665	3.588	13.638	1.00 46.99
ATOM	2030	CE	LYS .	A 317	51.165	2.686	12.514	1.00 48.65
ATOM	2031	NZ	LYS .	A 317	51.731	1.410	13.043	1.00 49.49
ATOM	2032	И		A 318	45.965	5.818	13.245	1.00 31.00
ATOM	2033	CA		A 318	45.188	6.272	14.408	1.00 30.33
MOTA	2034	C						
				A 318	44.683	5.120	15.263	1.00 30.57
MOTA	2035	0		A 318	44.171	4.088	14.732	1.00 29.80
MOTA	2036	CB		A 318	44.014	7.135	13.944	1.00 28.83
MOTA	2037	CG		A 318	44.436	8.367	13.197	1.00 28.31
MOTA	2038	CD1	PHE .	A 318	44.625	8.333	11.817	1.00 27.09
ATOM	2039			A 318	44.686	9.554	13.879	1.00 27.59
ATOM	2040			A 318	45.060	9.466	11.130	1.00 27.37
ATOM	2041			A 318	45.122	10.691	13.200	1.00 26.98
MOTA	2042	CZ		A 318	45.309	10.648	11.826	1.00 27.12
11 Ox1		U 2	~ 11£	1. 010	47.303	10,040	14.020	1.00 41.14

ATOM	2043	N	PRO I	A 319	44.805	5.252	16.591	1.00 30.02
ATOM	2044	CA	PRO 1	A 319	44.361	4.222	17.535	1.00 30.20
ATOM	2045.	С	PRO I	A 319	42.864	3.977	17.460	1.00 29.88
ATOM	2046	0		A 319	42.087	4.882	17.040	1.00 29.27
ATOM	2047	СВ		319	44.777	4.793	18.890	
ATOM	2048	CG						1.00 30.49
				1 319	44.667	6.276	18.674	1.00 31.99
ATOM .	2049	CD		1 319	45.308	6.437	17.309	1.00 30.77
ATOM	2050	N		320	42.449	2.779	17.860	1.00 30.08
ATOM	2051	CA	ASP I	A 320	41.018	2.389	17.867	1.00 29.79
ATOM	2052	С	ASP A	A 320	40.183	3.406	18.652	1.00 28.71
ATOM	2053	0		320	40.560	3.804	19.804	1.00 27.90
ATOM	2054	СВ	ASP A		40.855	1.009	18.520	1.00 27.30
ATOM	2055	CG	ASP A		41.545	-0.104	17.740	
ATOM	2056		ASP A					1.00 34.27
					41.787	-1.182	18.331	1.00 34.13
ATOM	2057		ASP A		41.833	0.092	16.538	1.00 35.41
ATOM	2058	N	GLY A		39.067	3.837	18.068	1.00 26.34
MOTA	2059	CA	GLY A		38.193	4.781	18.745	1.00 24.91
MOTA	2060	С	GLY A	321	38.439	6.259	18.490	1.00 23.96
MOTA	2061	0	GLY A	321	37.632	7.129	18.941	1.00 23.66
ATOM	2062	N	PHE A	322	39.519	6.591	17.793	1.00 22.07
ATOM	2063	CA	PHE A		39.810	8.011	17.507	1.00 20.41
ATOM	2064	C	PHE A		38.705	8.670		1.00 20.41
ATOM	2065	ō	PHE A				16.684	
ATOM	2066				38.157	9.743	17.078	1.00 20.75
		CB	PHE A		41.126	8.157	16.747	1.00 19.07
MOTA	2067	CG	PHE A		41.405	9.567	16.306	1.00 19.05
MOTA	2068	CD1			41.701	10.555	17.240	1.00 17.04
MOTA	2069		PHE A		41.326	9.918	14.960	1.00 17.20
MOTA	2070	CE1	PHE A	322	41.912	11.872	16.840	1.00 18.99
MOTA	2071	CE2	PHE A	322	41.535	11.229	14.552	1.00 17.99
ATOM	2072	CZ	PHE A		41.829	12.210	15.494	1.00 16.28
MOTA	2073	N	TRP A		38.367	8.063	15.552	1.00 20.75
ATOM	2074	CA	TRP A		37.330	8.622		
ATOM	2075	C	TRP A		35.940		14.664	1.00 22.37
		_				8.626	15.273	1.00 23.50
ATOM	2076	0.	TRP A		35.036	9.379	14.804	1.00 22.84
MOTA	2077	CB	TRP A		37.322	7.872	13.335	1.00 21.45
MOTA	2078	CG	TRP A		38.643	7.924	12.664	1.00 20.71
MOTA	2079	CD1			39.566	6.921	12.594	1.00 20.50
ATOM	2080	CD2	TRP A	323	39.217	9.049	11.986	1.00 20.31
ATOM	2081	NE1	TRP A	323	40.679	7.349	11.913	1.00 20.18
MOTA	2082	CE2	TRP A	323	40.492	8.651	11.527	1.00 20.95
MOTA	2083	CE3	TRP A	323	38.778	10.354	11.722	1.00 20.80
ATOM	2084	CZ2	TRP A		41.337	9.511	10.816	1.00 20.49
MOTA	2085		TRP A		39.618	11.212	11.013	1.00 21.58
ATOM	2086		TRP A		40.885	10.784	10.569	
ATOM	2087	N.	LEU A					1.00 21.15
ATOM	2088				35.734	7.810	16.300	1.00 26.13
		CA	LEU A		34.428	7.772	16.983	1.00 27.96
MOTA	2089	C	LEU A		34.417	8.877	18.040	1.00 29.09
MOTA	2090	0	LEU A		33.413	9.044	18.799	1.00 29.23
MOTA	2091	CB	LEU A	. 324	34.202	6.408	17.642	1.00 29.11
MOTA	2092	CG	LEU A	324	33.910	5.236	16.697	1.00 30.04
MOTA	2093	CD1	LEU A	324	33.791	3.948	17.501	1.00 30.31
MOTA	2094		LEU A		32.625	5.499	15.924	1.00 29.47
ATOM	2095	N	GLY A		35.513	9.634	18.098	1.00 29.34
ATOM	2096	CA	GLY A		35.632	10.728	19.048	
ATOM	2097	C	GLY A					1.00 30.68
					35.794	10.280	20.489	1.00 31.19
MOTA	2098	0	GLY A		35.687	11.109	21.442	1.00 31.53
MOTA	2099	N	GĻU A		36.067	8.995	20.683	1.00 32.22
MOTA	2100	CA	GLU A		36.225	8.436	22.042	1.00 34.09
ATOM	2101	С	GLU A		37.655	8.482	22.563	1.00 33.56
ATOM	2102	0	GLU A	326	37.907	8.933	23.720	1.00 34.19
ATOM	2103	CB	GLU A	326	35.728	6.992	22.062	1.00 35.56
MOTA	2104	CG	GLU A		34.267	6.847	21.683	1.00 38.03
						-		-

ATOM	2105	CD	GLU A	326	33.855	5.401	21.494	1.00 40.36
ATOM	2106	OE1	GLU A	326	32.662	5.162	21.207	1.00 41.84
MOTA	2107.	OE2	GLU A		34.720	4.506	21.626	
			-					1.00 42.10
MOTA	2108	N	GLN A		38.602	8.031	21.750	1.00 32.81
ATOM	2109	CA	GLN A	327	40.009	8.017	22.178	1.00 31.36
MOTA	2110	С	GLN A	327	40.844	9.142	21.608	1.00 30.14
ATOM	2111	0	GLN A	327	40.612	9.626	20.458	1.00 28.97
ATOM	2112	CB	GLN A		40.650	6.667	21.842	1.00 34.41
ATOM	2113	CG	GLN A		40.770	5.749	23.060	1.00 38.96
ATOM								
	2114	CD	GLN A		39.443	5.546	23.778	1.00 40.61
ATOM	2115		GLN A		39.410	5.223	25.002	1.00 42.73
MOTA	2116	NE2			38.344	5.714	23.053	1.00 42.75
ATOM	2117	N	LEU A	328	41.814	9.581	22.394	1.00 28.01
MOTA	2118	CA	LEU A	328	42.695	10.663	21.964	1.00 28.64
MOTA	2119	С	LEU A	328	43.889	10.100	21.219	1.00 27.50
ATOM	2120	0	LEU A		44.207	8.873	21.317	1.00 27.23
ATOM	2121	CB	LEU A		43.177	11.467	23.180	1.00 29.39
ATOM	2122	CG	LEU A		43.924	10.735	24.304	
								1.00 31.09
ATOM	2123		LEU A		45.298	10.283	23.831	1.00 31.75
MOTA	2124		LEU A		44.074	11.669	25.498	1.00 31.12
ATOM	2125	N	VAL A	329	44.539	10.961	20.449	1.00 25.26
MOTA	2126	CA	VAL A	329	45.748	10.583	19.722	1.00 23.64
MOTA	2127	С	VAL A	329	46.779	11.593	20.203	1.00 23.76
ATOM	2128	0	VAL A	329	46.431	12.786	20.476	1.00 21.96
ATOM	2129	СВ	VAL A		45.560	10.675	18.194	1.00 23.82
ATOM	2130		VAL A		45.100	12.070	17.794	1.00 23.64
ATOM	2131		VAL A		46.866	10.317	17.501	1.00 23.70
ATOM	2132	N	CYS A		48.025	11.157	20.344	1.00 23.69
MOTA	2133	CA	CYS A		49.088	12.046	20.830	1.00 24.17
MOTA	2134	C	CYS A	330	50.315	12.060	19.937	1.00 23.87
MOTA	2135	0	CYS A	330	50.592	11.089	19.165	1.00 24.32
MOTA	2136	СВ	CYS A	330	49.548	11.633	22.228	1.00 24.93
ATOM	2137	SG	CYS A	330	48.353	11.638	23.608	1.00 29.07
ATOM	2138	N	TRP A		51.069	13.144	20.047	1.00 22.66
ATOM	2139	CA	TRP A		52.306	13.318	19.281	1.00 22.40
ATOM	2140	C	TRP A		53.333			
						13.972	20.177	1.00 22.22
ATOM	2141	0	TRP A		52.979	14.698	21.154	1.00 21.57
MOTA	2142	CB	TRP A		52.069	14.207	18.064	1.00 21.16
MOTA	2143	CG	TRP A		51.345	13.524	16.959	1.00 19.61
MOTA	2144	CD1	TRP A	331	51.868	12.634	16.067	1.00 18.33
MOTA	2145	CD2	TRP A	331	49.966	13.684	16.606	1.00 18.42
MOTA	2146	NE1	TRP A	331	50.902	12.233	15.177	1.00 17.37
MOTA	2147	CE2	TRP A	331	49.721	12.862	15.488	1.00 18.60
ATOM	2148		TRP A		48.911	14.446	17.130	1.00 19.20
ATOM	2149		TRP A		48.467	12.778	14.874	1.00 17.86
ATOM	2150		TRP A		47.659	14.364	16.521	1.00 17.80
	2151							
MOTA			TRP A		47.450	13.535	15.406	1.00 19.08
MOTA	2152	N	GLN A		54.598	13.730	19.873	1.00 23.04
MOTA	2153	CA	GLN A		55.689	14.321	20.648	1.00 25.14
MOTA	2154	С	GLN A	332	55.490	15.836	20.594	1.00 23.64
MOTA	2155	0	GLN A	332	55.066	16.397	19.533	1.00 23.11
MOTA	2156	CB	GLN A	332	57.020	13.937	20.015	1.00 27.80
MOTA	2157	ĊG	GLN A		58.171	13.877	20.982	1.00 33.30
MOTA	2158	CD	GLN A		59.450	13.445	20.305	1.00 35.55
ATOM	2159		GLN A		60.060	14.224	19.507	1.00 36.94
ATOM	2160							1.00 36.57
			GLN A		59.879	12.217	20.579	
MOTA	2161	N	ALA A		55.778	16.506	21.704	1.00 22.79
MOTA	2162	CA	ALA A		55.618	17.977	21.820	1.00 21.04
MOTA	2163	С	ALA A		55.936	18.759	20.552	1.00 19.77
MOTA	2164	0	ALA A		57.076	18.671	19.997	1.00 19.85
MOTA	2165	CB	ALA A	333	56.475	18.499	22.971	1.00 21.00
MOTA	2166	N	GLY A	334	54.949	19.515	20.083	1.00 17.64

MOTA	2167	CA	GLY			55.123	20.340	18.903	1.00 16.89
MOTA	2168	С	GLY	Α	334	55.205	19.663	17.548	1.00 17.61
MOTA	2169.	0	GLY	A	334	55.403	20.370	16.512	1.00 17.50
MOTA	2170	N	THR	Α	335	55.060	18.343	17.490	1.00 16.55
MOTA	2171	CA	THR	Α	335	55.146	17.648	16.182	1.00 17.58
MOTA	2172	С	THR	Α	335	53.802	17.260	15.557	1.00 16.83
ATOM	2173	0	THR			53.761	16.408	14.618	1.00 17.71
ATOM	2174	СB	THR			56.017	16.377	16.275	1.00 17.71
ATOM	2175	OG1	THR			55.361	15.401	17.095	
ATOM	2176	CG2			•	57.373	16.710	16.884	1.00 17.56
ATOM	2177	N N	THR				17.842		1.00 17.23
						52.707		16.037	1.00 16.75
ATOM	2178	CA	THR			51.373	17.527	15.460	1.00 16.56
ATOM.	2179 ·	C	THR			51.473	17.752	13.952	1.00 16.24
MOTA	2180	0	THR			51.821	18.868	13.487	1.00 16.30
MOTA	2181	CB	THR			50.267	18.437	16.030	1.00 17.05
ATOM	2182	OG1	THR			50.181	18.255	17.451	1.00 17.15
MOTA	2183	CG2	THR			48.917	18.096	15.401	1.00 16.72
MOTA	2184	N	PRO			51.182	16.718	13.157	1.00 15.50
ATOM	2185	CA	PRO			51.254	16.820	11.699	1.00 14.87
MOTA	2186	С	PRO	A	337	50.006	17.444	11.082	1.00 14.56
MOTA	2187	0	PRO			49.310	16.800	10.249	1.00 14.49
ATOM	2188	CB	PRO	A	337	51.448	15.369	11.281	1.00 15.18
ATOM	2189	CG	PRO	A	337	50.520	14.657	12.238	1.00 16.05
MOTA	2190	CD	PRO	Α	337	50.784	15.359	13.572	1.00 15.54
MOTA	2191	N	TRP	Α	338	49.713	18.682	11.470	1.00 14.89
MOTA	2192	CA	TRP	Α	338	48.535	19.415	10.956	1.00 14.85
MOTA	2193	C	TRP	Α	338	48.339	19.304	9.445	1.00 14.87
ATOM	2194	0	TRP	Α	338	47.194	19.048	8.966	1.00 17.13
ATOM	2195	CB	TRP	Α	338	48.639	20.899	11.313	1.00 13.77
ATOM	2196	CG	TRP	Α	338	48.784	21.176	12.767	1.00 15.11
ATOM	2197	CD1				49.897	21.652	13.411	1.00 14.78
ATOM	2198	CD2	TRP			47.780	21.011	13.771	1.00 14.17
ATOM	2199	NE1	TRP			49.641	21.794	14.756	1.00 14.64
ATOM	2200	CE2				48.348	21.407	15.003	1.00 14.35
ATOM	2201	CE3	TRP			46.451	20.566	13.751	1.00 14.31
ATOM	2202	CZ2	TRP			47.635	21.371	16.202	1.00 14.86
ATOM	2203	CZ3	TRP			45.744	20.530	14.945	1.00 16.02
ATOM	2204	CH2	TRP			46.339	20.932	16.154	1.00 14.77
ATOM	2205	N	ASN			49.414	19.486	8.682	1.00 13.22
ATOM	2206	CA	ASN			49.319	19.449	7.203	1.00 13.22
ATOM	2207	C	ASN			48.674	18.208	6.608	1.00 12.01
ATOM	2208	ō	ASN			48.061	18.288	5.508	1.00 13.99
ATOM	2209	СВ	ASN			50.699	19.649	6.552	1.00 13.55
ATOM	2210	CG	ASN			51.576	18.404	6.627	1.00 15.28
ATOM	2211		ASN			52.290	18.174	7.648	1.00 16.29
MOTA	2212		ASN			51.541	17.584	5.578	1.00 12.93
ATOM	2213	N	ILE			48.774	17.064	7.276	1.00 12.93
ATOM	2214	CA	ILE			48.171		6.698	
ATOM	2215	C	ILE			46.655	15.831 15.864	6.794	1.00 12.98 1.00 12.80
ATOM	2216								
ATOM	2217	O CB	ILE			45.944	15.237	5.959	1.00 12.80 1.00 14.79
						48.667	14.545	7.400	
ATOM	2218		ILE			48.142	14.512	8.833	1.00 14.91
ATOM	2219		ILE			50.194	14.483	7.372	1.00 12.38
MOTA	2220		ILE			48.177	13.142	9.454	1.00 17.42
ATOM	2221	N	PHE			46.138	16.577	7.790	1.00 13.19
MOTA	2222		PHE			44.677	16.689	7.972	1.00 13.87
MOTA	2223	C	PHE			44.143	17.741	7.006	1.00 13.37
ATOM	2224	0	PHE			44.787	18.812	6.798	1.00 12.72
ATOM	2225	CB	PHE			44.354	17.087	9.410	1.00 13.10
ATOM	2226	CG	PHE			44.685	16.027	10.429	1.00 13.55
ATOM	2227		PHE			43.817	14.960	10.654	1.00 13.48
MOTA	2228	CD2	PHE	A	341	45.861	16.104	11.171	1.00 12.12

MOTA	2229	CE1	PHE A	341	44.115	13.984	11.607	1.00 13.44
MOTA	2230	CE2	PHE A	341	46.172	15.136	12.127	1.00 14.31
ATOM	2231	CZ	PHE A		45.298			
						14.074	12.346	1.00 13.92
ATOM	2232	N	PRO A	342	42.975	17.484	6.402	1.00 12.78
ATOM	2233	CA	PRO A	342	42.357	18.413	5.448	1.00 12.17
ATOM	2234	С	PRO A		41.565	19.544	6.100	1.00 12.90
ATOM	2235		PRO A					
		0		•	41.168	19.465	7.309	1.00 12.52
ATOM	2236	CB	PRO A	342	41.447	17.502	4.638	1.00 10.18
MOTA	2237	CG	PRO A	342	40.920	16.570	5.714	1.00 11.48
ATOM	2238	CD	PRO A		42.180	16.244	6.523	1.00 12.10
MOTA	2239	N	VAL A		41.342	20.609	5.342	1.00 12.27
ATOM	2240	CA	VAL A	343	40.528	21.712	5.851	1.00 10.51
MOTA	2241	С	VAL A	343	39.101	21.281	5.521	1.00 12.41
ATOM	2242	ō	VAL A					
					38.878	20.401	4.632	1.00 10.45
ATOM	2243	CB	VAL A		40.838	23.054	5.143	1.00 10.23
MOTA	2244	CG1	VAL A	343	42.247	23.507	5.488	1.00 8.58
MOTA	2245	CG2	VAL A	343	40.672	22.914	3.636	1.00 8.08
ATOM	2246	N	ILE A		38.132	21.848		
							6.224	1.00 13.49
MOTA	2247	CA	ILE A		36.725	21.507	5.991	1.00 13.17
ATOM	2248	С	ILE A	344	35.989	22.789	5.664	1.00 13.33
MOTA	2249	0	ILE A	344	36.067	23.795	6.427	1.00 13.12
MOTA	2250	CB	ILE A		36.099	20.859	7.246	1.00 14.77
MOTA	2251	CG1	ILE A		36.776	19.512	7.517	1.00 14.50
MOTA	2252	CG2	ILE A	344	34.585	20.702	7.060	1.00 13.14
MOTA	2253	CD1	ILE A	344	36.374	18.875	8.825	1.00 17.73
MOTA	2254	N	SER A	345	35.292	22.794	4.537	1.00 12.41
ATOM	2255	CA	SER A		34.547	23.982	4.136	1.00 13.41
MOTA	2256	C	SER A		33.051	23.723	4.172	1.00 14.94
MOTA	2257	0	SER A	345	32.555	22.641	3.721	1.00 14.55
ATOM	2258	CB	SER A	345	34.967	24.430	2.728	1.00 14.23
ATOM	2259	OG	SER A	345	36.329	24.834	2.703	1.00 13.57
MOTA	2260	N	LEU A		32.320	24.682	4.725	•
MOTA	2261	CA	LEU A		30.859	24.594	4.796	1.00 14.08
MOTA	2262	C	LEU A	346	30.320	25.772	4.003	1.00 13.86
ATOM	2263	0	LEU A	346	30.681	26.956	4.286	1.00 13.52
ATOM	2264	CB	LEU A	346	30.383	24.674	6.252	1.00 15.83
ATOM	2265	CG	LEU A		30.239	23.372	7.051	1.00 17.74
MOTA	2266		LEU A		31.455	22.492	6.875	1.00 18.92
MOTA	2267	CD2	LEU A		30.028	23.711	8.521	1.00 19.69
MOTA	2268	N	TYR A	347	29.496	25.485	3.000	1.00 13.48
ATOM	2269	CA	TYR A	347	28.894	26.543	2.176	1.00 13.76
MOTA	2270	C	TYR A		27.525	26.864	2.745	
								1.00 14.58
MOTA	2271	0	TYR A		26.676	25.948	2.979	1.00 13.16
MOTA	2272	CB	TYR A		28.757	26.101	0.716	1.00 14.82
MOTA	2273	CG	TYR A	347	30.066	26.051	-0.034	1.00 15.10
ATOM	2274	CD1	TYR A	347	31.022	25.074	0.252	1.00 13.97
MOTA	2275		TYR A		30.349	26.977	-1.038	1.00 13.98
MOTA	2276		TYR A		32.228	25.018	-0.447	1.00 14.47
MOTA	2277	CE2	TYR A	347	31.556	26.930	-1.746	1.00 15.69
ATOM	2278	cz	TYR A	347	32.487	25.949	-1.445	1.00 15.09
ATOM	2279	ОН	TYR A	347	33.672	25.895	-2.141	1.00 16.72
MOTA	2280	N	LEU A		27.288	28.145	2.971	1.00 13.86
MOTA	2281	CA	LEU A		26.018	28.593	3.545	1.00 16.70
MOTA	2282	С	LEU A		25.246	29.445	2.559	1.00 17.37
MOTA	2283	0	LEU A	348	25.856	30.183	1.722	1.00 16.05
ATOM	2284	СВ	LEU A		26.292	29.401	4.814	1.00 15.57
ATOM	2285	CG	LEU A		27.019	28.620	5.908	1.00 17.10
			LEU A					
MOTA	2286				27.518	29.565	6.985	1.00 15.71
MOTA	2287		LEU A		26.078	27.580	6.495	1.00 16.92
MOTA	2288	N	MET A	349	23.922	29.352	2.617	1.00 19.68
ATOM	2289	CA	MET A	349	23.073	30.167	1.734	1.00 22.78
ATOM	2290	C	MET A		23.384	31.629	2.024	1.00 22.03
		_			20.504		02-3	22.03

		_							
MOTA	2291	0	MET	Α	349	23.478	32.049	3.222	1.00 20.70
MOTA	2292	CB	MET	Α	349	21.594	29.897	2.008	1.00 25.40
MOTA	2293.	CG	MET	Α	349	20.931	28.954	1.012	1.00 31.18
ATOM	2294	SD	MET	Α	349	19.139	28.833	1.272	1.00 37.43
ATOM	2295	CE			349	18.697	30.583	1.318	
ATOM	2296	N			350				1.00 32.73
	2297	CA				23.573	32.414	0.972	1.00 20.81
ATOM					350	23.857	33.824	1.167	1.00 23.50
ATOM	2298	С			350	22.565	34.612	1.280	1.00 24.26
MOTA	2299	0	GLY	A	350	21.450	34.042	1.091	1.00 23.13
MOTA	2300	N	GLU	A	351	22.662	35.899	1.591	1.00 27.25
ATOM	2301	CA	GLU	A	351	21.448	36.734	1.698	1.00 32.00
ATOM	2302	С	GLU	Α	351	20.870	36.948	0.306	1.00 33.92
ATOM	2303	0			351	19.620	37.066	0.125	
ATOM	2304	ĊВ			351	21.774			1.00 34.42
ATOM	2305						38.081	2.340	1.00 32.31
		CG	GLU			22.012	37.996	3.831	1.00 34.92
ATOM	2306	CD			351	21.916	39.346	4.503	1.00 35.55
MOTA	2307	OE1				22.819	40.187	4.293	1.00 36.64
MOTA	2308	OE2	GLU	Α	351	20.927	39.567	5.233	1.00 36.29
ATOM	2309	N	VAL	Α	352	21.753	37.007	~0.684	1.00 36.98
ATOM	2310	CA	VAL	Α	352	21.327	37.181	~2.082	1.00 38.72
MOTA	2311	С	VAL	Α	352	20.944	35.809	-2.629	1.00 40.47
MOTA	2312	0	VAL			21.689	34.799	-2.426	1.00 39.68
ATOM	2313	СВ	VAL			22.456	37.767	-2.420	1.00 39.08
ATOM	2314		VAL			21.999			
							37.892	-4.382	1.00 38.33
MOTA	2315		VAL			22.866	39.123	-2.391	1.00 37.93
MOTA	2316	N	THR			19.806	35.747	-3.314	1.00 42.33
ATOM	2317	CA	THR			19.300	34.476	-3.882	1.00 43.97
ATOM	2318	С	THR	Α	353	20.254	33.832	-4.877	1.00 43.18
MOTA	2319	0	THR	Α	353	20.941	34.536	-5.688	1.00 42.65
ATOM	2320	CB	THR	A	353	17.929	34.672	-4.578	1.00 45.29
MOTA	2321	OG1				18.018	35.743	-5.526	1.00 46.63
ATOM	2322		THR			16.849	34.988	-3.551	1.00 46.31
ATOM	2323	N	ASN			20.307	32.507	-4.839	
ATOM	2324	CA	ASN						1.00 42.20
ATOM	2325					21.183	31.741	-5.742	1.00 43.39
		C	ASN			22.641	32.166	-5.611	1.00 41.22
MOTA	2326	0	ASN			23.444	32.078	-6.584	1.00 43.04
ATOM	2327	CB	ASN			20.698	31.887	-7.187	1.00 45.64
ATOM	2328	CG	ASN			19.467	31.036	-7.474	1.00 47.44
ATOM	2329		ASN			18.824	31.163	-8.562	1.00 48.61
MOTA	2330	ND2	ASN	Α	354	19.121	30.159	-6.534	1.00 47.73
MOTA	2331	N	GLN	Α	355	22.999	32.621	-4.419	1.00 37.62
ATOM	2332	CA	GLN	Α	355	24.371	33.042	-4.128	1.00 34.85
ATOM	2333	С	GLN	Α	355	24.737	32.475	-2.764	1.00 32.57
ATOM	2334	0	GLN			23.863	32.388	-1.846	1.00 31.25
ATOM	2335	CB	GLN			24.459	34.563	-4.105	1.00 31.23
ATOM	2336	CG	GLN			25.834			
ATOM	2337	CD	GLN				35.089	-3.797	1.00 38.04
						25.909	36.590	-3.915	1.00 39.05
ATOM	2338		GLN			25.586	37.171	-4.992	1.00 40.57
ATOM	2339		GLN .			26.331	37.249	-2.844	1.00 39.68
MOTA	2340	N	SER .			25.989	32.071	-2.597	1.00 29.33
MOTA	2341	CA	SER .	Α	356	26.419	31.514	-1.304	1.00 25.60
ATOM	2342	С	SER .	Α	356	27.850	31.897	-0.981	1.00 22.66
MOTA	2343	Ö	SER .	Α	356	28.580	32.481	-1.833	1.00 21.99
MOTA	2344	CB	SER .			26.313	29.991	-1.318	1.00 25.71
MOTA	2345	OG	SER .			27.449	29.425	-1.945	1.00 24.59
ATOM	2346	N	PHE .			28.267	31.583	0.239	1.00 20.53
ATOM	2347	CA	PHE .						
ATOM	2348	C				29.639	31.865	0.676	1.00 17.95
			PHE .			30.104	30.643	1.437	1.00 17.15
ATOM	2349	0	PHE .			29.279	29.750	1.784	1.00 17.21
MOTA	2350	CB	PHE .			29.687	33.126	1.550	1.00 17.62
MOTA	2351	CG	PHE :			28.926	33.017	2.850	1.00 17.61
MOTA	2352	CD1	PHE	A	357	29.571	32.625	4.018	1.00 15.09

ATOM	2353	CD2	PHE	7.	257	22 622	22 259	0.010	
ATOM	2354					27.577	33.357	2.912	1.00 16.90
			PHE			28.887	32.577	5.229	1.00 14.87
MOTA	2355	CE2			357	26.881	33.312	4.120	1.00 15.64
ATOM	2356	CZ			357	27.538	32.924	5.280	1.00 16.14
MOTA	2357	N			358	31.397	30.545	1.687	1.00 16.29
ATOM	2358	CA	ARG	Α	358	31.891	29.383	2.412	1.00 14.04
ATOM	2359	С	ARG	Α	358	32,642	29.755	3.664	1.00 14.59
ATOM	2360	0	ARG	Α	358	33.237	30.869	3.785	1.00 13.01
ATOM	2361	СВ			358	32.784	28.525	1.516	1.00 14.11
ATOM	2362	CG			358	34.084	29.172	1.102	
ATOM	2363	CD			358	34.809			1.00 13.28
						_	28.275	0.121	1.00 13.06
ATOM	2364	NE			358	36.090	28.831	-0.291	1.00 14.39
ATOM	2365	CZ			358	36.723	28.489	-1.409	1.00 14.92
ATOM	2366		ARG			36.188	27.591	-2.232	1.00 13.71
ATOM	2367	NH2	ARG	Α	358	37.888	29.045	-1.701	1.00 12.88
ATOM	2368	N	ILE	Α	359	32.612	28.819	4.596	1.00 14.51
ATOM	2369	CA	ILE	Α	359	33.268	28.935	5.891	1.00 16.36
MOTA	2370	С	ILE	Α	359	34.242	27.762	5.913	1.00 15.41
ATOM	2371	0			359	33.836	26.583	5.675	1.00 15.49
MOTA	2372	СВ			359	32.197	28.824	7.001	1.00 17.94
ATOM	2373	CG1			359	31.543	30.190	7.198	
ATOM	2374	CG2			359				1.00 19.68
ATOM	2375	CD1				32.766	28.260	8.255	1.00 20.12
						32.515	31.288	7.500	1.00 22.40
ATOM	2376	N			360	35.513	28.046	6.162	1.00 13.01
MOTA	2377	CA	THR			36.531	26.983	6.167	1.00 14.32
MOTA	2378	С			360	37.307	26.894	7.470	1.00 14.04
MOTA	2379 -	_	THR			37.892	27.913	7.938	1.00 13.82
MOTA	2380	CB	THR	Α	360	37.536	27.202	5.021	1.00 14.49
ATOM	2381	OG1	THR	Α	360	36.828	27.286	3.774	1.00 15.69
ATOM	23,82	CG2	THR	Α	360	38.532	26.053	4.964	1.00 15.11
ATOM	2383	N	ILE	Α	361	37.331	25.709	8.074	1.00 13.79
ATOM	2384	CA	ILE	Α	361	38.091	25.524	9.330	1.00 17.36
ATOM	2385	С	ILE	Α	361 .	39.241	24.548	9.122	1.00 16.53
MOTA	2386	0			361	39.237	23.717	8.160	1.00 16.37
ATOM	2387	CB			361	37.208	24.982	10.476	1.00 18.15
MOTA	2388	CG1	ILE			36.608	23.632		1.00 18.53
ATOM	2389	CG2	ILE			36.126	25.999	10.830	1.00 18.95
ATOM	2390	CD1	ILE			35.899	22.937	11.208	1.00 18.19
ATOM	2391	N	LEU			40.230	24.614	9.998	1.00 17.82
ATOM	2392	CA	LEU			41.375	23.710	9.876	
ATOM	2393	C	LEU			41.412			1.00 18.92
ATOM	2394	0	LEU			40.533	22.659 22.654	10.983	1.00 17.87
ATOM	2395							11.912	1.00 17.21
ATOM	2396	CB	LEU			42.675		9.837	1.00 22.47
		CG	LEU			42.686	25.974	10.320	1.00 25.03
MOTA	2397		LEU			42.945	25.992	11.802	1.00 28.14
MOTA	2398		LEU			43.781	26.751	9.623	1.00 25.06
MOTA	2399	N	PRO			42.380	21.729	10.910	1.00 16.12
ATOM	2400	CA	PRO			42.507	20.681	11.925	1.00 14.51
ATOM	2401	С	PRO			42.628	21.325	13.303	1.00 14.50
MOTA	2402	0	PRO			42.234	20.710	14.339	1.00 13.48
ATOM	2403	CB	PRO	Α	363	43.801	19.971	11.534	1.00 15.57
ATOM	2404	CG	PRO	Α	363	43.902	20.202	10.076	1.00 16.87
ATOM	2405	CD	PRO	Α	363	43.450	21.616	9.903	1.00 14.60
ATOM	2406	N	GLN	Α	364	43.178	22.539	13.337	1.00 12.36
MOTA	2407	CA	GLN	Α	364	43.357	23.271	14.608	1.00 13.04
ATOM	2408	С	GLN			42.014	23.557	15.254	1.00 13.41
MOTA	2409	0	GLN			41.953	23.895	16.467	1.00 12.73
ATOM	2410	CB	GLN			44.111	24.585	14.392	1.00 12.04
ATOM	2411	CG	GLN			45.637	24.449	14.304	1.00 11.85
ATOM	2412	CD	GLN			46.141	24.079	12.919	1.00 11.11
ATOM	2413		GLN			47.372	24.211	12.625	1.00 13.65
ATOM	2414	NE2				45.245	23.621	12.056	1.00 8.04
		*****				- J.64J	23.021	. 2.000	2.00 .0.04

			~		265	40 000			
MOTA	2415	N	GLŅ			40.939	23.446	14.478	1.00 13.30
MOTA	2416	CA	GLN	Α	365	39.580	23.657	15.023	1.00 14.36
MOTA	2417	С	GLN	Α	365	38.873	22.341	15.339	1.00 14.57
ATOM	2418	0	GLN			38.312	22.175	16.457	1.00 16.56
ATOM	2419	СВ	GLN			38.691	24.452		
								14.056	1.00 14.03
MOTA	2420	CG	GLN			38.816	25.962	14.167	
MOTA	2421	CD	GLN	Α	365	40.073	26.489	13.515	1.00 15.81
MOTA	2422	OE1	GLN	Α	365	40.290	26.292	12.282	1.00 15.51
ATOM	2423	NE2	GLN	Α	365	40.917	27.158	14.295	1.00 15.82
ATOM	2424	N	TYR			38.873	21.392	14.406	1.00 14.93
ATOM	2425	CA			366	38.149		14.673	
							20.128		1.00 15.12
ATOM	2426	C			366	38.914		15.447	1.00 15.66
MOTA	2427	0	TYR			38.378	17.930	15.703	1.00 17.42
ATOM	2428	CB	TYR	Α	366	37.557	19.567	13.371	1.00 14.28
MOTA	2429	CG	TYR	Α	366	38.541	19.107	12.322	1.00 13.05
MOTA	2430	CD1	TYR	A	366	39.228	17.907	12.467	1.00 13.67
ATOM	2431	CD2	TYR	Α	366	38.721	19.835	11.145	1.00 13.44
ATOM	2432	CE1				40.062	17.431	11.463	1.00 12.91
ATOM	2433	CE2				39.555	19.369	10.128	1.00 12.63
ATOM	2434	CZ	TYR						_
						40.218	18.163	10.294	1.00 13.86
MOTA	2435	OH	TYR			41.008	17.669	9.287	1.00 12.42
ATOM	2436	N	LEU			40.144	19.367	15.835	1.00 16.84
MOTA	2437	CA	LEU	Α	367	40.966	18.450	16.660	1.00 16.98
ATOM	2438	С	LEU	Α	367	40.996	19.161	18.017	1.00 17.50
ATOM	2439	0	LEU	Α	367	41.662	20.224	18.172	1.00 16.40
MOTA	2440	CB	LEU			42.382	18.324	16.088	1.00 17.44
ATOM	2441	CG	LEU			42.764	16.991	15.429	1.00 18.54
ATOM	2442		LEU			41.681	16.534	14.482	1.00 17.60
MOTA	2443		LEU			44.091	17.143	14.700	1.00 17.38
ATOM	2444	N	ARG			40.270	18.624	18.990	1.00 17.06
MOTA	2445	CA	ARG	Α	368	40.192	19.253	20.326	1.00 17.22
MOTA	2446	С	ARG	Α	368	41.341	18.874	21.243	1.00 16.52
MOTA	2447	0	ARG	Α	368	41.554	17.662	21.538	1.00 16.19
MOTA	2448	CB	ARG			38.879	18.871	21.009	1.00 16.02
ATOM	2449	CG	ARG			38.050	20.055	21.444	1.00 19.09
ATOM	2450	CD	ARG			37.415	19.811	22.792	1.00 17.88
			ARG						
ATOM	2451	NE				36.840	18.474	22.906	1.00 17.20
MOTA	2452	CZ	ARG			36.775	17.806	24.053	1.00 18.65
ATOM	2453		ARG			37.247	18.361	25.164	1.00 18.77
ATOM	2454	NH2	ARG	Α	368	36.258	16.584	24.095	1.00 17.53
ATOM	2455	N	PRO	Α	369	42.100	19.867	21.722	1.00 17.88
MOTA	2456	CA	PRO	Α	369	43.220	19.558	22.615	1.00 19.69
ATOM	2457	С	PRO	Α	369	42.744	19.067	23.969	1.00 22.16
ATOM	2458	0			369	41.786	19.645	24.575	1.00 20.49
ATOM	2459	СВ			369	43.983	20.883	22.700	1.00 20.03
	2460	CG			369		21.911	22.429	1.00 19.96
ATOM						42.932			
MOTA	2461	CD			369	42.122	21.285	21.320	1.00 17.42
ATOM	2462	N	VAL			43.376	18.001	24.444	1.00 23.75
MOTA	2463	CA	VAL	A	370	43.040	17.399	25.747	1.00 27.84
MOTA	2464	С	VAL	Α	370	44.332	16.921	26.394	1.00 30.26
MOTA	2465	0	VAL	Α	370	45.321	16.577	25.682	1.00 30.79
ATOM	2466	CB	VAL	Α	370	42.093	16.197	25.577	1.00 26.52
ATOM	2467		VAL			40.771	16.654	24.989	1.00 26.57
ATOM	2468		VAL			42.737	15.160	24.669	1.00 26.53
	2469	N	GLU					27.719	1.00 20.55
MOTA						44.361	16.891		
MOTA	2470	CA	GLU			45.574	16.450	28.426	1.00 40.60
ATOM	2471	С	GLU			45.800	14.963	28.235	1.00 42.42
ATOM	2472	0	GLU			44.832	14.138	28.321	1.00 41.89
ATOM				_	271	45 470	16 750	20 021	1 00 40 10
AIOM	2473	CB	GLU	A	3/1	45.472	16.758	29.921	1.00 43.12
MOTA		CB CG	GLU GLU			45.472	17.634	30.443	1.00 43.12
MOTA	2473			A	371				
	2473 2474	CG CD	GLU	A A	371 371	46.603	17.634	30.443	1.00 47.33

ATOM	2477	OE2	CT.II	7	371	48.710	10 151	00 456	
ATOM	2478						18.151	29.456	1.00 51.00
		N			372	47.046	14.596	27.960	1.00 45.77
ATOM	2479.	CA			372	47.396	13.182	27.774	1.00 49.75
MOTA	2480	С			372	46.889	12.468	29.014	1.00 52.41
ATOM	2481	0	ASP	A	372	47.090	12.966	30.165	1.00 52.32
MOTA	2482	CB	ASP	Α	372	48.913	13.015	27.665	1.00 50.28
MOTA	2483	CG			372	49.323	11.587	27.333	1.00 51.15
ATOM	2484		ASP			50.541			
ATOM	2485		ASP				11.323	27.246	1.00 51.32
						48.429	10.729	27.156	1.00 50.76
MOTA	2486	N			373	46.217	11.340	28.819	1.00 55.35
MOTA	2487	CA			373	45.688	10.570	29.956	1.00 58.73
MOTA	2488	С	VAL	Α	373	46.850	10.213	30.896	1.00 60.04
·MOTA	2489 ·	0	VAL	Α	373	47.465	9.105	30.817	1.00 60.06
ATOM	2490	CB	VAL	Α	373	44.901	9.313	29.433	1.00 59.43
MOTA	2491	CGI	VAL			45.292	8.044	30.176	1.00 59.64
MOTA	2492		VAL			43.402	9.556	29.597	
ATOM	2493	N			374				1.00 59.89
ATOM						47.187	11.169	31.759	1.00 61.58
	2494	CA			374	48.277	11.020	32.755	1.00 61.52
ATOM	2495	С			374	49.709	11.205	32.233	1.00 61.38
MOTA	2496	0			374	50.104	10.633	31.169	1.00 60.95
MOTA	2497	CB	ALA	Α	374	48.155	9.668	33.455	1.00 62.66
MOTA	2498	N	THR	Α	375	50.477	12.002	32.977	1.00 61.03
ATOM	2499	CA	THR	Α	375	51.919	12.320	32.715	1.00 60.30
ATOM	2500	С			375	52.401	12.358	31.269	1.00 58.41
ATOM	2501	Ō			375	52.361	11.308		
ATOM	2502	СВ			375			30.555	1.00 59.21
						52.838	11.327	33.455	1.00 61.35
MOTA	2503	OG1				52.302	11.049	34.756	1.00 62.26
ATOM	2504	CG2	THR			54.237	11.912	33.599	1.00.61.47
ATOM	2505	N			376	52.892	13.520	30.833	1.00 55.18
ATOM	2506	CA	SER	Α	376	53.407	13.683	29.445	1.00 51.40
MOTA	2507	С	SER	Α	376	53.538	15.132	28.981	1.00 48.79
MOTA	2508	0	SER	Α	376	52.887	16.067	29.540	1.00 48.19
MOTA	2509	CB			376	52.502	12.943	28.456	1.00 51.90
MOTA	2510	OG			376	52.880	13.193	27.115	1.00 51.90
ATOM	2511	N	GLN			54.373	15.333		
ATOM	2512	CA	GLN					27.968	1.00 44.88
ATOM	2513	C				54.576	16.664	27.367	1.00 41.28
			GLN			54.106	16.580	25.923	1.00 37.22
MOTA	2514	0	GLN		_	54.380	17.489	25.081	1.00 35.23
ATOM	2515	CB	GLN			56.048	17.062	27.425	1.00 43.59
MOTA	2516	CG	GLN			56.468	17.585	28.789	1.00 46.22
MOTA	2517	$^{\rm CD}$	GLN			57.955	17.831	28.886	1.00 47.12
MOTA	2518	OE1	GLN	A	377	58.710	17.710	27.867	1.00 48.44
MOTA	2519	NE2	GLN	Α	377	58.414			1.00 48.23
ATOM	2520	N	ASP			53.399	15.499	25.618	1.00 31.89
ATOM '	2521	CA	ASP			52.866	15.289	24.263	1.00 28.31
ATOM	2522	C	ASP			51.663	16.183	24.034	1.00 25.36
ATOM	2523	ō	ASP						
MOTA	2524	СВ				50.958	16.590	25.004	1.00 22.58
MOTA			ASP			52.422	13.835	24.072	1.00 28.64
	2525	CG	ASP			53.582	12.867	23.998	1.00 29.19
MOTA	2526		ASP			54.746	13.316	23.948	1.00 30.91
ATOM	2527	OD2	ASP	A	378	53.323	11.647	23.981	1.00 30.50
MOTA	2528	N	ASP	Α	379	51.415	16.513	22.776	1.00 23.06
MOTA	2529	ĊA	ASP	Α	379	50.236	17.317	22.436	1.00 22.51
MOTA	2530	С	ASP			49.220	16.294	21.964	1.00 21.46
MOTA	2531		ASP			49.436	15.581	20.945	1.00 19.87
ATOM	2532	СВ	ASP			50.570			
ATOM	2533	CG	ASP				18.335	21.346	1.00 21.72
ATOM	2534					51.557	19.377	21.829	1.00 23.29
			ASP			51.434	19.786	23.005	1.00 23.00
ATOM	2535		ASP			52.446	19.789	21.052	1.00 23.50
ATOM	2536	N	CYS			48.128	16.182	22.706	1.00 20.99
ATOM	2537	CA	CYS			47.082	15.201	22.393	1.00 20.40
MOTA	2538	С	CYS	A	380	45.769	15.865	22.013	1.00 19.94
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ATOM	_	0	CYS			45.489	17.038	22.417	1.00 18.77
ATOM	2540	CB	CYS	A	380	46.867	14.292	23.596	1.00 23.14
MOTA	2541	SG	CYS	Α	380	48.368	13.550	24.327	1.00 25.25
ATOM	2542	N	TYR			44.947			
							15.140	21.255	1.00 18.49
ATOM	2543	CA	TYR	A.	381	43.656	15.681	20.785	1.00 17.31
ATOM	2544	С	TYR	Α	381	42.595	14.610	20.602	1.00 17.45
MOTA	2545	0	TYR	Δ	381	42.890	13.376	20.532	1.00 16.46
		-							
MOTA	2546	CB	TYR			43.833	16.370	19.427	1.00 15.47
ATOM	2547	CG	TYR	Α	381	45.034	17.275	19.314	1.00 14.93
ATOM	2548	CD1	TYR	Ά	381	44.899	18.659	19.408	1.00 14.20
ATOM	2549								
			TYR			46.311	16.746	19.118	1.00 14.17
MOTA	2550	CE1	TYR	A	381	46.009	19.499	19.307	1.00 14.66
MOTA	2551	CE2	TYR	Α	381	47.431	17.576	19.021	1.00 15.73
ATOM	2552	CZ	TYR	Δ	381	47.272	18.952	19.113	1.00 16.02
ATOM						•			
	2553	OH	TYR			48.369	19.785	18.994	1.00 15.32
ATOM	2554	N	LYS	A	382	41.356	15.066	20.506	1.00 18.35
MOTA	2555	CA	LYS	Α	382	40.218	14.174	20.248	1.00 20.26
MOTA	2556	С	LYS			39.555	14.695	18.981	1.00 19.31
MOTA	2557	0	LYS			39.575	15.941	18.704	1.00 19.65
MOTA	2558	CB	LYS			39.221	14.204	21.404	1.00 21.74
ATOM	2559	CG	LYS	Α	382	39.632	13.348	22.585	1.00 25.42
MOTA	2560	CD	LYS			38.509	13.266	23.602	1.00 27.59
ATOM	2561	CE	LYS			38.878	12.342	24.759	1.00 29.84
MOTA	2562	NZ	LYS	Α	382	37.779	12.246	25.761	1.00 31.22
ATOM	2563	N	PHE	Α	383	38.994	13.786	18.192	1.00 18.55
MOTA	2564	CA	PHE	Δ	383	38.298	14.165	16.942	1.00 16.97
ATOM	2565								
		C	PHE			36.992	14.823	17.375	1.00 16.22
ATOM	2566	0	PHE	А	383	36.079	14.138	17.908	1.00 13.73
MOTA	2567	CB	PHE	Α	383	38.026	12.907	16.110	1.00 16.57
MOTA	2568	CG	PHE	Α	383	37.447	13.182	14.750	1.00 16.49
ATOM	2569		PHE			38.052	14.091	13.890	1.00 14.48
MOTA	2570		PHE			36.319	12.489	14.308	1.00 15.06
ATOM	2571	CE1	PHE	Α	383	37.542	14.306	12.606	1.00 16.02
MOTA	2572	CE2	PHE	Α	383	35.807	12.696	13.029	1.00 15.64
ATOM	2573	CZ	PHE			36.419	13.603	12.176	1.00 15.10
ATOM	2574								
		N	ALA			36.885	16.134	17.173	1.00 16.28
ATOM	2575	CA	ALA			35.675	16.893	17.586	1.00 15.54
ATOM	2576	С	ALA	Α	384	34.549,	16.931	16.559	1.00 15.46
ATOM	2577	0	ALA	Α	384	33.768	17.931	16.487	1.00 15.60
ATOM	2578	CB	ALA			36.061	18.316	17.987	1.00 14.96
MOTA	2579	N	ILE			34.451	15.888	15.745	1.00 14.66
MOTA	2580	CA	ILE	Α	385	33.356	15.792	14.763	1.00 13.45
MOTA	2581	С	ILE	Α	385	32.651	14.487	15.093	1.00 14.39
ATOM	2582	0	ILE			33.303	13.410	15.179	1.00 12.37
ATOM	2583	CB	ILE			33.862			
							15.724	13.315	1.00 12.54
MOTA	2584		ILE			34.696	16.959	12.988	1.00 13.08
ATOM	2585	CG2	ILE	Α	385	32.675	15.655	12.367	1.00 12.56
ATOM	2586	CD1	ILE	A	385	35.178	17.003	11.549	1.00 10.74
ATOM	2587	N	SER				14.543		
						31.343		15.297	1.00 14.95
MOTA	2588	CA	SER			30.605	13.319	15.637	1.00 16.99
MOTA	2589	С	SER	Α	386	29.275	13.221	14.918	1.00 17.48
ATOM	2590	0	SER	Α	386	28.795	14.207	14.279	1.00 18.09
MOTA	2591	СВ	SER			30.385	13.240	17.151	1.00 16.69
MOTA	2592	OG	SER			29.630	14.345	17.616	1.00 16.81
MOTA	2593	N ·	GLN			28.673	12.044	15.016	1.00 19.86
MOTA	2594	CA	GLN	Α	387	27.384	11.748	14.376	1.00 23.09
АТОМ	2595	С	GLN			26.209	12.317	15.160	1.00 22.61
MOTA	2596		GLN			26.221	12.363	16.427	1.00 22.90
ATOM	2597								
			GLN			27.222	10.234		1.00 24.53
MOTA	2598		GLN			26.035	9.795	13.411	1.00 28.94
MOTA	2599	CD	GLN	Α	387	25.971	8.286	13.272	1.00 30.39
MOTA	2600		GLN			27.013	7.619	12.999	1.00 31.54
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3.000	2621		~	_						
MOTA	2601	NE2	GLN	Α	387	24.782	7.721	13.441	1.00	32.07
MOTA	2602	N	SER	Α	388	25.186	12.743	14.434		21.60
ATOM	2603	CA	SER	Α	388	23.981	13.306			
ATOM	2604							15.055		21.59
		С			388	22.728	12.711	14.429	1.00	22.68
ATOM	2605	0	SER	Ά	388	22.707	12.380	13.203	1.00	23.08
ATOM	2606	СВ	SER	Α	388'	23.959	14.824	14.871		
ATOM	2607	OG								19.88
					388	22.661	15.342	15.112	1.00	19.18
ATOM	2608	N	SER	Α	389	21.681	12.551	15.227	1,00	23.51
ATOM	2609	CA	SER	Ά	389	20.405	12.024	14.690		
ATOM	2610	С								24.44
					389	19.391	13.167	14.708	1.00	23.83
ATOM	2611	0	SER	Α	389	18.181	12.973	14.385	1.00	23.81
ATOM	2612	CB	SER	Α	389	19.902	10.847	15.534		25.63
ATOM	2613	OG			389	19.681				
							11.235	16.881	1.00	27.65
ATOM	2614	N	THR			19.861	14.360	15.066	1.00	22.66
MOTA	2615	CA	THR	Α	390	18.984	15.553	15.127		22.60
ATOM	2616	С	THR			19.471	16.709			
ATOM	2617	ō						14.260		21.12
			THR			19.272	17.910	14.608	1.00	21.35
MOTA	2618	CB	THR	Α	390	18.825	16.052	16.577	1.00	23.02
ATOM	2619	OG1	THR	Α	390	20.117	16.288	17.150		24.55
MOTA	2620	CG2								
ATOM						18.079	15.010	17.413		23.83
	2621	N	GLY			20.093	16.381	13.136	1.00	19.75
MOTA	2622	CA	GLY	Α	391	20.573	17.410	12.237		16.88
ATOM	2623	С	GLY	Δ	391	21.982	17.891	12.526		
ATOM	2624									17.24
		0	GLY			22.672	17.402	¹ 13.472	1.00	16.27
ATOM	2625	N	THR	Α	392	22.427	18.851	11.730	1.00	14.99
ATOM	2626	CA	THR	Α	392	23.773	19.423	11.880	1.00	
ATOM	2627	C	THR							
						23.841	20.514	12.938	1.00	
ATOM	2628	0	THR			22.949	21.409	13.012	1.00	16.11
MOTA	2629	CB	THR	Α	392	24.266	20.062	10.564	1.00	
MOTA	2630	OG1	THR			24.494	19.043	9.588		
ATOM	2631								1.00	
		CG2	THR			25.572	20.839	10.800	1.00	14.09
MOTA	2632	N	VAL	Α	393	24.857	20.458	13.779	1.00	13.06
MOTA	2633	CA	VAL	A	393	25.027	21.534	14.746	1.00	
ATOM	2634	С	VAL			26.462				
							22.033	14.684	1.00	15.47
MOTA	2635	0	VAL			27.450	21.265	14.908	1.00	16.85
ATOM	2636	СВ	VAL	A	393	24.619	21.128	16.201	1.00	16.35
ATOM	2637	CG1	VAL	Α	393	24.559	19.624	16.348	1.00	
MOTA	2638		VAL							
						25.566	21.766	17.210	1.00	13.79
MOTA	2639	N	MET			26.592	23.298	14.312	1.00	15.41
ATOM	2640	CA	MET	Α	394	27.900	23.962	14.231	1.00	16.55
ATOM	2641	С	MET	Α	394	28.188	24.442	15.647		
ATOM	2642	ō	MET						1.00	
		_				27.737	25.553	16.059	1.00	
ATOM	2643	CB	MET	A,	394	27.822	25.143	13.264	1.00	16.88
ATOM	2644	CG	MET	A	394	27.607	24.724	11.818	1.00	
ATOM	. 2645	SD	MET			27.178	26.083	10.700	1.00	
MOTA	2646	CE								
			MET			25.475	25.768	10.522	1.00	
MOTA	2647	N	GLY	A	395	28.909	23.622	16.406	1.00	16.28
ATOM	2648	CA	GLY .	Α	395	29.220	23.967	17.780	1.00	
ATOM	2649	С	GLY .			30.487				
ATOM							24.775	17.971	1.00	
	2650	0	GLY			31.011	25.408	17.005	1.00	16.25
MOTA	2651	N	ALA .	Α	396	30.989	24.769	19.202	1.00	17.29
ATOM	2652	CA	ALA .			32.211	25.511	19.586	1.00	
ATOM	2653	C	ALA							
						33.383	25.310	18.634	1.00	
ATOM	2654	0	ALA .			34.050	26.303	18.223	1.00	22.56
MOTA	2655	CB	ALA .	A	396	32.626	25.128	21.013	1.00	
MOTA	2656	N	VAL .			33.661	24.065	18.269		
ATOM	2657								1.00	
		CA	VAL .			34.792	23.781	17.353	1.00	
ATOM	2658	С	VAL :			34.690	24.592	16.068	1.00	21.89
MOTA	2659	0	VAL .	A	397	35.731	25.029	15.496	1.00	
ATOM	2660	СВ	VAL			34.874	22.274	17.012		
ATOM									1.00	44.19
	2661		VAL			35.065	21.480	18.287	1.00	
MOTA	2662	CG2	VAL 2	A.	397	33.623	21.826	16.290	1.00 2	

3.0014	2662		TT - 200				
MOTA	2663		ILE A 398	33.472		15.586	1.00 21.78
MOTA	2664	CA	ILE A 398	33.276	25.612	14.359	1.00 21.50
ATOM	2665	. C	ILE A 398	33.403		14.735	1.00 19.91
ATOM	2666	0	ILE A 398	34.222			
ATOM	2667				-	14.135	1.00 16.77
			ILE A 398	31.872	25.390	13.749	1.00 23.48
MOTA	2668			31.859	24.113	12.910	1.00 26.70
ATOM	2669	CG2	ILE A 398	31.469	26.596	12.895	1.00 24.67
ATOM	2670	CD1	ILE A 398	32.656	24.223	11.620	
ATOM	2671	N	MET A 399				1.00 27.64
				32.614	27.492	15.726	1.00 17.64
ATOM	2672	CA	MET A 399	32.594	28.889	16.201	1.00 16.99
MOTA	2673	С	MET A 399	33.951	29.439	16.640	1.00 17.65
ATOM	2674	0	MET A 399	34.202	30.677	16.517	1.00 18.70
MOTA	2675	СВ	MET A 399	31.575			
ATOM	2676				29.025	17.331	1.00 15.33
		CG	MET A 399	30.138	28.800	16.866	1.00 14.30
MOTA	2677	SD	MET A 399	28.891	29.038	18.155	1.00 16.41
ATOM	2678	CE	MET A 399	28.972	30.826	18.388	1.00 10.15
ATOM	2679	N	GLU A 400	34.835	28.579	17.143	
ATOM	2680	CA	GLU A 400				1.00 16.09
ATOM	2681			36.175	29.051	17.580	1.00 16.46
		С	GLU A 400	36.968	29.576	16.389	1.00 14.50
ATOM	2682	0	GLU A 400	37.971	30.332	16.553	1.00 14.83
MOTA	2683	CB	GLU A 400	36.957	27.919	18.257	1.00 15.95
ATOM	2684	CG	GLU A 400	36.318	27.419	19.540	
ATOM	2685	CD	GLU A 400				1.00 18.44
				37.156	26.376	20.243	1.00 18.72
MOTA	2686		GLU A 400	37.771	25.542	19.546	1.00 20.29
MOTA	2687	OE2	GLU A 400	37.186	26.383	21.493	1.00 19.60
ATOM	2688	N	GLY A 401	36.544	29.204	15.190	1.00 13.62
ATOM	2689	CA	GLY A 401	37.246	29.662	14.010	
ATOM	2690	C	GLY A 401				1.00 15.09
				36.747	31.010	13.533	1.00 16.28
ATOM	2691	0	GLY A 401	37.435	31.693	12.716	1.00 16.14
ATOM	2692	N	PHE A 402	35.591	31.438	14.033	1.00 14.90
ATOM	2693	CA	PHE A 402	35.018	32.712	13.572	1.00 15.01
ATOM	2694	С	PHE A 402	34.378	33.605		
ATOM	2695	ŏ				14.615	1.00 15.52
			PHE A 402	34.078	33.185	15.7 7 7	1.00 16.47
ATOM	2696	CB	PHE A 402	33.966	32.424	12.495	1.00 14.48
ATOM	2697	CG	PHE A 402	34.381	31.364	11.522	1.00 15.64
ATOM	2698	CD1	PHE A 402	34.126	30.021	11.785	1.00 14.91
ATOM	2699	CD2		35.095	31.700	10.376	1.00 15.20
MOTA	2700		PHE A 402		20.000		
				34.581	29.027	10.920	1.00 15.18
ATOM	2701		PHE A 402	35.555	30.717	9.507	1.00 15.72
MOTA	2702	CZ	PHE A 402	35.298	29.376	9.782	1.00 15.12
ATOM	2703	N	TYR A 403	34.168	34.847	14.208	1.00 15.73
ATOM	2704	CA	TYR A 403	33.474	35.837	15.039	1.00 15.81
ATOM	2705	C	TYR A 403	32.071			
ATOM	2706				35.641	14.489	1.00 14.48
		0	TYR A 403	31.846	35.789	13.250	1.00 15.47
ATOM	2707	CB	TYR A 403	33.977	37.251	14.731	1.00 14.45
ATOM	2708	CG	TYR A 403	33.265	38.340	15.499	1.00 15.22
MOTA	2709	CD1	TYR A 403	32.899	38.152	16.834	1.00 14.85
ATOM	2710		TYR A 403	33.018			
ATOM	2711		TYR A 403		39.584	14.916	1.00 14.28
				32.311	39.175	17.569	1.00 15.25
MOTA	2712		TYR A 403	32.435	40.617	15.644	1.00 14.12
ATOM	2713	CZ	TYR A 403	32.086	40.406	16.967	1.00 15.72
ATOM	2714	OH	TYR A 403	31.525	41.427	17.697	1.00 18.09
ATOM	2715	N	VAL A 404	31.125			
ATOM	2716				35.286	15.345	1.00 14.70.
			VAL A 404	29.753	35.040	14.854	1.00 14.44
MOTA	2717		VAL A 404	28.759	36.079	15.342	1.00 14.92
MOTA	2718		VAL A 404	28.552	36.259	16.582	1.00 15.62
ATOM	2719	CB	VAL A 404	29.284	33.629	15.260	1.00 14.39
ATOM	2720		VAL A 404	27.925	33.323		
ATOM	2721		VAL A 404			14.640	1.00 11.90
				30.327	32.603	14.819	1.00 12.73
ATOM	2722		VAL A 405	28.136	36.762	14.386	1.00 16.06
ATOM	2723		VAL A 405	27.153	37.822	14.676	1.00 14.31
ATOM	2724	С	VAL A 405	25.717	37.312	14.562	1.00 16.79

MOTA	2725	0	VAL	A	405	25.238	36.955	13.443	1.00	16.14
MOTA	2726	CB	VAL	A	405	27.318	39.004	13.700		13.66
ATOM	2727		VAL			26.302	40.092	14.021		12.39
MOTA	2728	CG2	VAL	Α	405	28.739	39.547	13.775		10.80
MOTA	2729	N			406	25.019	37.260	15.691		16.73
MOTA	2730	CA	PHE	Α	406	23.616	36.805	15.685		16.73
ATOM	2731	С	PHE			22.755	38.049	15.531		17.47
ATOM	2732	0	PHE	Α	406	22.286	38.654	16.539		17.39
MOTA	2733	СВ	PHE			23.287	36.053	16.979		13.96
MOTA	2734	ÇG	PHE			24.061	34.765	17.139		13.82
MOTA	2735	CD1	PHE			25.398	34.783	17.533		13.31
ATOM	2736		PHE			23.464	33.538	16.863		12.85
MOTA	2737		PHE			26.128	33.601	17.646		13.23
MOTA	2738	CE2				24.185	32.350	16.973		12.78
ATOM	2739	CZ	PHE			25.522	32.382	17.367		12.76
ATOM	2740	N	ASP .			22.566	38.449	14.278		18.08
MOTA	2741	CA	ASP			21.785	39.647	13.932		19.70
ATOM	2742	С	ASP			20.297	39.316	13.927		19.73
ATOM	2743	0	ASP .	Α	407	19.675	39.120	12.837		18.96
MOTA	2744	CB	ASP .	A	407	22.221	40.153	12.552		22.61
ATOM	2745	CG	ASP .			21.663	41.530	12.223		24.28
ATOM	2746		ASP .			20.660	41.935	12.849		24.12
MOTA	2747	OD2	ASP .			22.225	42.198	11.325		23.37
MOTA	2748	N	ARG .			19.709	39.245	15.116		19.72
MOTA	2749	CA	ARG .	A	408	18.269	38.928	15.259		22.01
MOTA	275 0	С	ARG :	A	408	17.393	39.967	14.557		21.56
ATOM	2751	0	ARG .	A	408	16.386	39.606	13.875		20.49
ATOM	2752	CB	ARG .			17.909	38.835	16.748		23.44
ATOM	2753	CG	ARG .			18.670	37.724	17.479		25.61
MOTA	2754	CD	ARG I			18.838	37.994	18.973		28.14
MOTA	2755	NE	ARG 2			17.843	37.328	19.814		31.17
ATOM	2756	CZ	ARG I			16.567	37.679	19.887		32.24
MOTA	2757		ARG I			16.127	38.693	19.163	1.00	35.70
ATOM	2758		ARG 2			15.735	37.029	20.687	1.00	31.13
ATOM	2759	И	ALA A			17.750	41.241	14.694		21.10
ATOM ATOM	2760	CA	ALA A			16.978	42.329	14.056		22.43
ATOM	2761 2762	С 0	ALA A			16.785	42.050	12.571		22.80
ATOM	2762	СВ	ALA A			15.646	42.177	12.034		24.04
ATOM	2764	N	ALA A			17.689	43.664	14.247		20.85
ATOM	2765	CA	ARG A			17.858	41.664	11.889		23.89
ATOM	2766	C	ARG A			17.770	41.374	10.445		25.07
ATOM	2767	õ	ARG A			17.639 17.908	39.888	10.119		24.26
ATOM	27 6 8	СВ	ARG I			18.987	39.461			24.63
ATOM	2769	CG	ARG A			19.025	41.949 43.464	9.724		26.83
ATOM	2770	CD	ARG A			19.326		9.700		29.89
ATOM	2771	NE	ARG A			20.590	44.664	8.295		32.69
MOTA	2772	CZ	ARG A			21.182	44.979	8.208 7.062		33.51 34.58
ATOM	2773		ARG A			20.626	44.631	5.907		33.99
MOTA	2774		ARG A			22.328	45.644	7.068		35.27
ATOM	2775	N	LYS A			17.223	39.091	11.097	1.00	
ATOM	2776	CA	LYS F			17.061	37.630	10.891		22.77
MOTA	2777	C	LYS A			18.227	37.031	10.104	1.00	
MOTA	2778	0	LYS A			18.015	36.309	9.081		20.39
MOTA	2779	СВ	LYS F			15.761	37.335	10.138	1.00	
MOTA	2780	CG	LYS A			14.491	37.686	10.136		23.33 27.80
MOTA	2781	CD	LYS A			13.270	37.188	10.121	1.00	
ATOM	2782	CE	LYS A			13.337	35.678	9.890	1.00	
ATOM	2783	NZ	LYS A			12.153	35.163	9.142	1.00	
MOTA	2784	N	ARG A			19.449	37.290	10.541	1.00	
MOTA	2785	CA	ARG A		412	20.607	36.748	9.815	1.00	
MOTA	2786	С	ARG A		412	21.789	36.505	10.736	1.00	
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ATOM	2787	0	ARG A	412	21.911	37.137	11.837	1.00 18.56
ATOM	2788	СВ	ARG A	412	21.019	37.714	8.703	1.00 18.72
	2789.	CG	ARG A					
MOTA			_		21.571	39.027	9.239	1.00 18.66
MOTA	2790	CD	ARG A	412	21.941	39.988	8.127	1.00 18.34
ATOM	2791	NE	ARG A	412	22.560	41.196	8.662	1.00 19.28
ATOM	2792	CZ	ARG A	412	23.082	42.163	7.916	1.00 20.03
	2793	NH1	ARG A		23.059			
MOTA						42.067	6.591	1.00 19.36
ATOM	2794	NHZ	ARG A		23.635	43.219	8.496	1.00 19.27
MOTA	2795	N	ILE A	413	22.668	35.606	10.317	1.00 17.01
ATOM	2796	CA	ILE A	413	23.865	35.285	11.103	1.00 16.43
ATOM	2797	C	ILE A		25.103	35.576	10.266	1.00 16.20
ATOM	2798	0	ILE A		25.213	35.125	9.084	1.00 17.17
MOTA	2799	СВ	ILE A	413	23.855	33.808	11.533	1.00 16.02
ATOM	2800	CG1	ILE A	413	22.667	33.562	12.469	1.00 13.92
ATOM	2801	CG2	ILE A	413	25.168	33.458	12.218	1.00 15.95
ATOM	2802	CD1	ILE A		22.482	32.130	12.862	1.00 14.89
MOTA	2803	N	GLY A		26.028	36.332	10.841	1.00 15.43
ATOM	2804	CA	GLY A	414	27.243	36.679	10.132	1.00 14.42
MOTA	2805	С	GLY A	414	28.463	35.899	10.585	1.00 14.91
ATOM	2806	0	GLY A	414	28.569	35.463	11.779	1.00 12.74
ATOM	2807	N	PHE A		29.392	35.709	9.656	1.00 12.70
MOTA	2808	CA	PHE A		30.638	34.977	9.932	1.00 14.84
ATOM	2809	С	PHE A	415	31.823	35.766	9.403	1.00 15.05
ATOM	2810	0	PHE A	415	31.761	36.376	8.291	1.00 17.34
ATOM	2811	CB	PHE A	415	30.613	33.599	9.256	1.00 13.57
ATOM	2812	CG	PHE A		29.628	32.640	9.860	1.00 13.35
MOTA	2813	CD1			30.034	31.710	10.820	1.00 14.56
MOTA	2814	CD2	PHE A	415	28.296	32.660	9.472	1.00 11.54
MOTA	2815	CE1	PHE A	415	29.117	30.809	11.383	1.00 13.74
MOTA	2816	CE2	PHE A	415	27.373	31.768	10.027	1.00 12.67
	2817	CZ	PHE A		27.787	30.839		
ATOM							10.985	1.00 13.15
MOTA	2818	N	ALA A		32.895	35.779	10.178	1.00 15.11
MOTA	2819	CA	ALA A	416	34.135	36.470	9.786	1.00 14.57
MOTA	2820	С	ALA A	416	35.248	35.738	10.515	1.00 14.48
MOTA	2821	0	ALA A		35.027	35.186	11.639	1.00 12.56
ATOM	2822	CB	ALA A		34.095	37.935	10.208	1.00 11.46
MOTA	2823	N	VAL A		36.425	35.692	9.906	1.00 14.71
MOTA	2824	CA	VAL A		37.569	35.011	10.528	1.00 16.80
MOTA	2825	C	VAL A	417	37.835	35.634	11.892	1.00 18.08
MOTA	2826	0	VAL A	417	37.922	36.901	12.033	1.00 17.13
ATOM	2827	СВ	VAL A		38.824	35.126	9.642	1.00 17.67
			VAL A					
MOTA	2828				40.022	34.486	10.333	1.00 16.83
MOTA	2829	CG2	VAL A		38.561	34.441	8.301	1.00 18.32
MOTA	2830	N	SER A	418	37.953	34.785	12.905	1.00 17.31
MOTA	2831	CA	SER A	418	38.201	35.271	14.272	1.00 17.62
MOTA	2832	С	SER A		39.637	35.712	14.455	1.00 18.36
ATOM	2833	ō	SER A		40.591	35.038	13.963	1.00 19.44
MOTA	2834	CB	SER A		37.882	34.182	15.295	1.00 18.09
ATOM	2835	OG	SER A	418	38.228	34.617	16.599	1.00 17.42
ATOM	2836	N	ALA A	419	39.821	36.827	15.150	1.00 17.60
MOTA	2837	CA	ALA A		41.175	37.335	15.410	1.00 18.46
	2838	C	ALA A		41.877	36.423	16.423	1.00 19.09
MOTA								
MOTA	2839	Ö	ALA A		43.117	36.553	16.649	1.00 19.60
MOTA	2840	CB	ALA A	419	41.106	38.772	15.943	1.00 17.70
ATOM	2841	N	CYS A	420	41.132	35.500	17.032	1.00 19.36
MOTA	2842	CA	CYS A		41.736	34.575	18.029	1.00 20.89
ATOM	2843	C	CYS A		41.677	33.105	17.624	1.00 19.60
ATOM	2844	0	CYS A		41.805	32.202	18.501	1.00 22.74
MOTA	2845	CB	CYS A		41.064	34.734	19.410	1.00 21.69
MOTA	2846	SG	CYS A	420	39.353	34.096	19.526	1.00 25.02
MOTA	2847	N	HIS A		41.495	32.814	16.342	1.00 17.86
ATOM	2848	CA	HIS A		41.435	31.393	15.933	1.00 17.71
111 011	20.0	CA	יידט ע					2.00 X/./1

MOTA	2849			A 421	42.834	30.798	15.799	1.00 17.18
ATOM	2850		HIS	A 421	43.801		15.356	
MOTA	2851		HIS.	A 421	40.641		14.625	1.00 18.65
MOTA	2852	CG	HIS	A 421	41.433		13.381	1.00 18.05
ATOM	2853	ND:	1 HIS		42.114	30.514	12.705	
MOTA	2854		2 HIS .		41.631			1.00 18.84
MOTA	2855		L HIS		42.695		12.678	1.00 18.73
ATOM	2856	NE			42.418		11.637	1.00 17.98
ATOM	2857	N		A 422			11.597	1.00 20.03
MOTA	2858	CA		A 422	42.965	29.533	16.194	
ATOM	2859	C		A 422	44.260		16.132	1.00 16.89
ATOM	2860	o			44.571	28.334	14.719	1.00 17.53
ATOM	2861	CB		A 422	43.678	27.764	14.021	1.00 17.13
ATOM	2862			A 422	44.257	27.588	17.061	1.00 16.92
ATOM	2863	CGI			45.632	26.938	17.063	1.00 15.15
ATOM		CG2			43.850	28.004	18.479	1.00 19.33
ATOM	2864	N	HIS A		45.815	28.531	14.291	1.00 16.64
ATOM	2865	CA	HIS A		46.264	28.112	12.940	1.00 16.92
ATOM	2866	C	HIS A		47.792	28.038	12.906	1.00 17.46
-	2867	0	HIS A		48.461	28.105	13.981	1.00 17.20
MOTA	2868	CB	HIS A		45.755	29.111	11.889	1.00 15.85
ATOM	2869	CG	HIS A		46.242	30.512	12.096	1.00 18.62
ATOM	2870		HIS A		47.390	30.998	11.504	1.00 19.80
ATOM	2871		HIS A		45.758	31.522	12.857	1.00 17.42
ATOM	2872		HIS A		47.590	32.245	11.892	1.00 18.22
ATOM	2873	NE2			46.615	32.586	12.714	1.00 18.53
ATOM	2874	N	ASP A		48.360	27.869	11.714	1.00 18.00
ATOM	2875	CA	ASP A		49.836	27.817	11.556	1.00 17.75
ATOM	2876	С	ASP A		50.194	28.804	10.453	1.00 18.36
MOTA	2877	0	ASP A	424	49.294	29.527	9.935	1.00 20.02
ATOM	2878	CB	ASP A	424	50.305	26.396	11.206	1.00 18.00
MOTA	2879	CG	ASP A		49.545	25.791	10.037	1.00 19.08
MOTA	2880	OD1	ASP A	424	49.110	24.623	10.149	1.00 18.99
MOTA	2881	OD2	ASP A	424	49.390	26.473	9.003	1.00 20.46
MOTA	2882	N	GLU A	425	51.459	28.877	10.063	1.00 20.40
MOTA	2883	CA	GLU A	425	51.813	29.853	9.015	1.00 17.33
ATOM	2884	C	GLU A	425	51.497	29.379	7.601	1.00 16.95
ATOM	2885	0	GLU A	425	51.724	30.131	6.613	1.00 17.24
MOTA	2886	CB	GLU A	425	53.289	30.239	9.112	1.00 17.24
MOTA	2887	CG	GLU A	425	54.254	29.150	8.714	1.00 20.84
ATOM	2888	CD	GLU A	425	55.632	29.697	8.381	1.00 20.84
MOTA	2889	OE1	GLU A		56.481	28.901	7.936	1.00 21.89
ATOM	2890	OE2	GLU A		55.867	30.920	8.559	1.00 22.65
ATOM	2891	N	PHE A	426	50.955	28.171	7.476	1.00 22.65
MOTA	2892	CA	PHE A		50.619	27.606	6.150	1.00 13.51
MOTA	2893	С	PHE A		49.157	27.767	5.763	1.00 15.51
ATOM	2894	0	PHE A		48.826	27.822	4.540	1.00 15.14
MOTA	2895	CB	PHE A		51.001	26.127	6.109	1.00 14.53
MOTA	2896	CG	PHE A		52.452	25.877	6.400	
ATOM	2897	CD1	PHE A		53.433	26.244	5.482	1.00 14.20
MOTA	2898		PHE A		52.841	25.298	7.606	1.00 13.59
MOTA	2899		PHE A		54.787	26.040	5.762	1.00 14.11
ATOM	290.0	CE2	PHE A	426	54.192	25.087		1.00 14.83
MOTA	2901	CZ	PHE A		55.167	25.460	7.897	1.00 15.49
ATOM	2902	N	ARG A		48.269	27.827	6.969	1.00 14.08
MOTA	2903	CA	ARG A		46.824	27.985	6.752	1.00 13.77
MOTA	2904	C	ARG A		46.130		6.469	1.00 14.89
ATOM	2905	ō	ARG A		46.630	28.695	7.615	1.00 15.43
ATOM	2906	CB	ARG A		46.132	28.710	8.781	1.00 14.58
MOTA	2907	CG	ARG A		46.959	26.632	6.301	1.00 15.33
ATOM	2908	CD	ARG A		46.645	25.518	5.707	1.00 16.84
ATOM	2909	NE	ARG A		45.994	24.234	6.477	1.00 17.68
MOTA	2910	CZ	ARG A		45.701	23.230	5.655	1.00 16.69
			.m.c A	341	42.10T	21.998	6.062	1.00 15.45

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MOTA	2911		ARG			45.114	21.159	5.224	1.00 14.20
MOTA	2912	NH2	ARG	Α	427	45.981	21.603	7.296	1.00 13.31
ATOM	2913	N	THR	Α	428	44.976	29.269	7.317	1.00 15.28
ATOM	2914	CA	THR	Α	428	44.180	29.967	8.336	1.00 17.94
MOTA	2915	С	THR			42.731	29.650	8.041	1.00 16.25
ATOM	2916	ō	THR			42.400	29.165	6.923	
			THR						1.00 14.77
ATOM .	2917	CB				44.353	31.503	8.249	1.00 18.18
ATOM	2918		THR			44.043	31.942	6.921	1.00 20.24
MOTA	2919	CG2	THR			45.773	31.901	8.583	1.00 19.84
MOTA	2920	N	ALA	Α	429	41.860	29.901	9.009	1.00 16.14
ATOM	2921	CA	ALA	A	429	40.423	29.677	8.803	1.00 16.03
ATOM	2922	С	ALA	Α	429	40.048	30.739	7.775	1.00 15.66
ATOM	2923	0	ALA	Α	429	40.808	31.738	7.574	1.00 14.51
ATOM	2924	СВ	ALA			39.656	29.898	10.105	1.00 17.08
ATOM	2925	N	ALA			38.920	30.575	7.107	1.00 14.04
ATOM	2926	CA	ALA			38.556	31.576	6.100	
									1.00 13.71
ATOM	2927	C	ALA			37.067	31.706	5.883	1.00 11.98
MOTA	2928	0	ALA			36.271	30.754	6.166	1.00 12.33
ATOM	2929	СВ	ALA			39.251	31.246	4.762	1.00 12.27
ATOM	2930	N	VAL		-	36.671	32.874	5.396	1.00 11.01
ATOM	2931	CA	VAL	Α	431	35.260	33.149	5.076	1.00 13.39
MOTA	2932	С	VAL	Α	431	35.344	33.773	3.697	1.00 15.69
ATOM	2933	0	VAL	Α	431	35.857	34.926	3.533	1.00 17.86
MOTA	2934	СВ	VAL.	Α	431	34.624	34.145	6.056	1.00 11.50
ATOM	2935		VAL			33.148	34.294	5.737	1.00 10.61
ATOM	2936		VAL			34.818	33.659	7.494	1.00 10.71
ATOM		N	GLU			34.874	33.048	2.694	1.00 16.74
ATOM	2938	CA	GLU			34.969	33.544	1.320	1.00 18.65
ATOM	2939	C	GLU			33.681	33.414	0.530	1.00 18.40
ATOM	2940	0	GLU			32.794	32.567	0.852	1.00 16.40
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MOTA	2941	CB	GLU			36.097	32.796	0.607	1.00 19.91
ATOM	2942	CG	GLU			37.460	33.031	1.241	1.00 24.66
ATOM	2943	CD	GLU			38.466	31.930	0.935	1.00 27.80
ATOM	2944		GLU			39.681	32.196	1.051	1.00 30.84
ATOM	2945		GLU			38.049	30.799	0.595	1.00 28.87
ATOM	2946	N	GLY			33.574	34.243	-0.504	1.00 18.95
MOTA	2947	CA	GLY			32.408	34.244	-1.363	1.00 19.36
MOTA	2948	С	GLY	Α	433	32.504	35.385	-2.359	1.00 19.59
ATOM	2949	0	GLY	A	433	33.489	36.173	-2.328	1.00 18.33
MOTA	2950	N	PRO	Α	434	31.511	35.539	-3.243	1.00 19.47
ATOM	2951	CA	PRO	Α	434	30.345	34.655	-3.285	1.00 19.72
ATOM	2952	С	PRO	Α	434	30.485	33.589	-4.353	1.00 19.98
ATOM	2953	0	PRO	Α	434	31.382	33.674	-5.235	1.00 22.24
ATOM	2954	CB	PRO			29.215	35.619	-3.595	1.00 19.80
ATOM	2955	CG	PRO			29.869	36.517	-4.616	1.00 19.70
ATOM	2956	CD	PRO			31.261	36.770	-4.018	1.00 19.73
АТОЙ	2957	N	PHE			29.624	32.583	-4.290	1.00 21.45
АТОМ	2958	CA	PHE			29.619	31.502	-5.292	1.00 22.31
ATOM	2959	C	PHE			28.217	31.513	-5.872	1.00 24.39
ATOM	2960	0	PHE			27.207	31.636	-5.110	1.00 24.58
ATOM	2961				435	29.924			
		CB					30.155	-4.636	1.00 22.02
MOTA	2962	CG	PHE			31.215	30.141	-3.876	1.00 20.80
MOTA	2963		PHE			31.232	30.392	-2.507	1.00 20.70
ATOM	2964		PHE			32.424	29.945	-4.542	1.00 21.70
ATOM	2965		PHE			32.432	30.451	-1.809	1.00 20.27
MOTA	2966		PHE			33.634	30.003	-3.853	1.00 21.68
ATOM	2967	CZ	PHE			33.637	30.259	-2.481	1.00 21.51
ATOM	2968	N	VAL	A	436	28.117	31.396	-7.192	1.00 27.02
MOTA	2969	CA	VAL	Α	436	26.802	31.438	-7.872	1.00 29.79
MOTA	2970	С	VAL	A	436	26.526	30.219	-8.739	1.00 32.85
MOTA	2971	0	VAL	A	436	25.434	30.120	-9.376	1.00 33.81
MOTA	2972	CB	VAL	A	436	26.702	32.677	-8.787	1.00 28.98

ATOM	2072	001	***		426				
	2973		VAL			26.999	33.944	-7.996	1.00 29.00
MOTA	2974	CG2	VAL	A	436	27.678	32.537	-9.947	1.00 28.49
MOTA	2975	N	THR	Α	437	27.473	29.292	-8.795	1.00 36.05
MOTA	2976	CA	THR			27.305	28.089	-	
ATOM	2977	C						-9.638	1.00 39.30
			THR			26.582	26.979	-8.870	1.00 41.99
MOTA	2978	0	THR	Α	437	26.604	25.775	-9.276	1.00 41.77
MOTA	2979	CB	THR	Α	437	28.690		-10.123	1.00 39.02
MOTA	2980	0G1	THR			28.552		-11.408	
ATOM	2981	CG2							1.00 42.51
						29.280	26.578	-9.156	1.00 38.10
MOTA	2982	N	LEU			25.908	27.368	-7.794	1.00 45.33
ATOM	2983	CA	LEU	Α	438	25.199	26.417	-6.901	1.00 49.22
ATOM	2984	С	LEU	Α	438	23.753	26.016	-7.165	
MOTA	2985	0	LEU			22.869			1.00 50.49
ATOM	2986						26.878	-7.466	1.00 51.99
		CB	LEU			25.276	26.944	-5.473	1.00 50.30
MOTA	2987	CG	LEU			26.027	28.269	-5.358	1.00 50.73
ATOM	2988	CD1	LEU	Α	438	25.108	29.457	-5.584	1.00 50.27
ATOM	2989		LEU			26.629	28.328	-4.001	1.00 51.67
ATOM	2990	N	ASP						
ATOM	2991					23.505	24.715	-7.037	1.00 52.67
		CA	ASP			22.149	24.128	-7.172	1.00 55.74
MOTA	2992	С	ASP			21.690	24.224	-5.722	1.00 56.96
MOTA	2993	0	ASP	Α	439	21.757	23.221	-4.945	1.00 57.33
MOTA	2994	CB	ASP	Α	439	22.240	22.657	-7.586	1.00 56.39
ATOM	2995	CG	ASP			20.879			
ATOM	2996						21.993	-7.695	1.00 57.68
			ASP			20.046	22.178	-6.781	1.00 57.75
ATOM	2997	OD2				20.645	21.274	-8.692	1.00 58.18
MOTA	2998	N	MET	Α	440	21.233	25.407	-5.337	1.00 58.71
ATOM	2999	CA	MET			20.841	25.656	-3.944	1.00 60.87
ATOM	3000	C	MET						
						19.435	26.215	-3.713	1.00 62.52
ATOM	3001	0	MET			19.247	27.451	-3.489	1.00 63.93
ATOM	3002	CB	MET			21.916	26.569	-3.346	1.00 60.48
ATOM	3003	CG	MET	Α	440	21.523	27.456	-2.201	1.00 60.72
ATOM	3004	SD	MET			22.755	28.755	-2.086	1.00 59.28
ATOM	3005	CE	MET						
ATOM						22.367	29.689	-3.543	1.00 59.46
	3006	N	GLU			18.435	25.343	-3.765	1.00 63.61
ATOM	3007	CA	GLU			17.042	25.774	-3.514	1.00 65.54
ATOM	3008	С	GLU	Α	441	16.356	24.847	-2.518	1.00 64.49
MOTA	3009	0	GLU			15.998	25.285	-1.375	1.00 65.36
ATOM	3010	СВ	GLU			16.229			
MOTA	3011						25.847	-4.815	1.00 67.99
		CG	GLU			16.500	24.745	-5.822	1.00 70.98
ATOM	3012	CD	GLU			17.353	25.228	-6.981	1.00 72.23
MOTA	3013	OE1	GLU	Α	441	18.507	25.646	-6.742	1.00 73.24
ATOM	3014	OE2	GLU	Α	441	16.867	25.194	-8.132	1.00 73.30
MOTA	3015	N	ASP			16.170	23.585		
MOTA	3016	CA	ASP						1.00 61.29
ATOM	3017					15.519	22.616	-1.986	1.00 58.37
		G.	ASP			16.504	21.966	-1.018	1.00 55.47
MOTA	3018	0	ASP			16.615	20.704	-0.950	1.00 54.59
MOTA	3019	CB	ASP	A	442	14.800	21.530	-2.785	1.00 59.93
MOTA	3020	CG	ASP			13.298	21.616	-2.646	1.00 60.90
ATOM	3021		ASP			12.689			
ATOM		001	ADF .	~	442		22.478	-3.312	1.00 61.34
	3022		ASP			12.729	20.832	-1.854	1.00 61.81
ATOM	3023	N	CYS	Α	443	17.207	22.790	-0.252	1.00 51.31
MOTA	3024	CA	CYS	Α	443	18.200	22.281	0.713	1.00 47.79
ATOM	3025	C	CYS .			17.635	22.156		1.00 46.40
ATOM	3026	ō	CYS					2.121	
ATOM						18.168	21.373	2.965	1.00 44.04
	3027	CB	CYS			19.421	23.198	0.713	1.00 48.61
ATOM	3028	SG	CYS .	Α	443	20.176	23.339	-0.939	1.00 46.95
MOTA	3029	N	GLY .	Α	444	16.566	22.895	2.395	1.00 45.40
ATOM	3030	CA	GLY .			15.953	22.846	3.709	1.00 45.06
ATOM	3031	C	GLY .			15.011			
ATOM	3032						21.673	3.899	1.00 45.25
		0	GLY .			14.271	21.264	2.952	1.00 44.97
ATOM	3033	N	TYR .			15.018	21.109	5.101	1.00 44.97
ATOM	3034	CA	TYR .	Α	445	14.140	19.968	5.421	1.00 44.48
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MOTA	3035	С	TYR	Α	445		12.778	20.467	5.882	1.00 45.23
ATOM	3036	0	TYR	Α	445		12.662	21.558	6.530	1.00 44.57
ATOM	3037	СВ	TYR	Α	445		14.801	19.172	6.531	1.00 43.11
ATOM	3038	CG	TYR				13.918			
								17.997	6.871	1.00 42.75
MOTA	3039	CD1					13.846	16.905	6.010	1.00 42.58
MOTA	3040	CD2	TYR	Α	445		13.170	17998	8.049	1.00 42.27
ATOM	3041	CE1	TYR	Α	445		13.042	15.820	6.327	1.00 41.99
ATOM	3042	CE2	TYR	Δ	445		12.358	16.917	8.360	1.00 43.20
ATOM	3043	CZ	TYR							
							12.289	15.835	7.503	1.00 41.98
MOTA	3044	ОН	TYR				11.490	14.751	7.810	1.00 20.00
MOTA	3045	N	ASN	Α	446		11.746	19.699	5.550	1.00 45.69
MOTA	3046	CA	ASN	Α	446		10.359	20.012	5.947	1.00 48.64
ATOM.	3047.	С	ASN	Δ	446		9.776	18.726	6.524	1.00 50.90
MOTA	3048	ō	ASN				9.894	17.625		
		_							5.896	1.00 51.59
ATOM	3049	CB	ASN				9.537	20.470	4.738	1.00 48.19
ATOM	3050	CG	ASN	A	446		9.975	21.827	4.213	1.00 48.18
MOTA	3051	OD1	ASN	Α	446		9.926	22.858	4.950	1.00 48.63
ATOM	3052	ND2	ASN	Α	446		10.403	21.867	2.957	1.00 48.04
ATOM	3053	N	ILE				9.165	18.826	7.700	1.00 53.94
ATOM	3054	CA	ILE				8.569			
								17.650	8.388	1.00 55.99
ATOM	3055	С	ILE				7.720	16.772	7.463	1.00 57.01
ATOM	3056	0	ILE	Α	447		7.449	17.195	6.318	1.00 58.11
ATOM	3057	CB	ILE	Α	447		7.699	18.105	9.577	1.00 55.86
MOTA	3058	CG1	ILE	Α	447		8.488	19.086	10.450	1.00 56.28
MOTA	3059	CG2	ILE				7.267	16.900	10.406	1.00 56.92
	3060									
ATOM		CD1					9.759	18.505	11.037	1.00 55.79
MOTA	3061	OXT	ILE		447		7.328	15.666	7.895	1.00 57.55
MOTA	3062	N	SER	P	1		35.528	15.672	28.238	1.00 37.61
MOTA	3063	CA	SER	P	1		34.172	16.082	28.590	1.00 36.72
ATOM	3064	С	SER	P	1		33.508	16.863	27.450	1.00 34.75
MOTA	3065	Ö	SER		ī		34.132			
								17.643	26.742	1.00 36.46
ATOM	3066	CB	SER		1		34.248	16.949	29.848	1.00 37.77
MOTA	3067	OG	SER	P	1		33.152	17.865	29.853	1.00 40.82
ATOM	3068	N	GLU	P	2		32.203	16.601	27.257	1.00 32.86
MOTA	3069	CA	GLU	Р	2		31.513	17.216	26.129	1.00 32.80
MOTA	3070	С	GLU	P	2		30.218	17.906	26.552	1.00 31.23
ATOM	3071	ō	GLU		2		29.435	17.401		
									27.348	1.00 31.31
MOTA	3072	CB	GLU	_	2		31.275.	16.167	25.027	1.00 33.64
MOTA	3073	CG	GLU	P	2		31.096	17.096	23.826	1.00 37.41
MOTA	3074	CD	GLU	P	2		31.076	15.940	22.852	1.00 38.37
MOTA	3075	OE1	GLU	P	2	:	31.996	15.134	22.983	1.00 39.04
ATOM	3076	OE2	GLU	р	2		30.175	15.798	22.037	1.00 39.43
ATOM	3077	N	VAL		3		29.742	19.344	26.106	1.00 27.98
	3078									
ATOM		CA	VAL		3		28.367	19.820	26.101	1.00 26.44
MOTA	3079	С	VAL		3		27.717	19.598	24.735	1.00 26.26
ATOM	3080	0	VAL	P	3		28.371	19.580	23.701	1.00 25.48
MOTA	3081	CB	VAL	P	3		28.377	21.311	26.429	1.00 25.89
ATOM	3082	CG1	VAL		3		28.684	21.516	27.911	1.00 27.07
ATOM	3083		VAL		3		29.431	22.012	25.594	1.00 23.97
MOTA	3084	N	ASN		4		26.361	19.591	25.174	1.00 25.89
MOTA	3085	CA	ASN		4		25.421	19.254	24.075	1.00 26.64
ATOM	3086	С	ASN	Ρ	4	:	24.027	19.825	24.452	1.00 26.87
MOTA	3087	0	ASN	P	· 4		23.116	19.163	25.077	1.00 27.10
MOTA	3088	СВ	ASN		4		25.349	17.766	23.876	1.00 27.95
ATOM	3089	CG	ASN		4		26.498			
								17.245	22.971	1.00 29.39
MOTA	3090		ASN		4		26.499	17.409	21.723	1.00 31.90
ATOM	3091	ND2	ASN		4		27.489	16.617	23.603	1.00 31.97
MOTA	3092	N	STA	P	5	:	24.115	21.101	24.323	1.00 25.26
MOTA	3093	CA	STA		5		22.965	21.865	24.929	1.00 25,83
ATOM	3094	СВ	STA		5		23.683	22.681	26.021	1.00 27.28
ATOM	3095	CG	STA		5		24.378	22.057	27.197	1.00 28.07
MOTA	3096	CDI	STA	2	5	•	25.002	23.077	28.182	1.00 27.46

30016	3005			_	_				
ATOM	3097				5	23.280	21.130	27.828	1.00 25.47
ATOM	3098	CH	STA	₽	5	22.223	22.851	23.940	1.00 25.86
MOTA	3099	OH	STA	P	5	23.028	23.679	23.298	1.00 25.23
ATOM	3100	CM	STA	P	5	21.372	21.980	23.048	
ATOM	3101	C	STA		5	20.420			1.00 27.11
ATOM							21.340	24.125	1.00 27.81
	3102	0	STA		5	20.241	20.065	24.095	1.00 25.70
MOTA	3103	N	VAL	P	6	19.339	22.479	23.764	1.00 26.04
ATOM	3104	CA	VAL	P	6	18.037	21.953	24.156	1.00 27.12
ATOM	3105	С	VAL		6	17.496	20.965		
ATOM	3106	ō	VAL		6			23.121	1.00 27.36
						17.795	21.029	21.936	1.00 26.97
ATOM	3107	CB	VAL		6	17.073	23.130	24.312	1.00 27.18
MOTA	3108	CG1	VAL	P	6	16.433	23.463	22.965	1.00 26.70
ATOM	3109	CG2	VAL	P	6	15.985	22.781	25.311	1.00 28.74
MOTA	3110	N	ALA	P	7	16.702	19.998	23.617	1.00 28.68
ATOM	3111	CA	ALA		7	16.158			
ATOM	3112	C	ALA		7		18.986	22.720	1.00 32.14
						14.774	19.377	22.197	1.00 32.99
MOTA	3113	0	ALA		7	14.040	20.149	22.801	1.00 32.08
MOTA	3114	CB	ALA	Ρ	7	16.072	17.666	23.489	1.00 31.38
MOTA	3115	N	GLU	P	8	14.443	18.843	21.007	1.00 36.10
MOTA	3116	CA	GLU	P	8	13.144	19.143	20.418	1.00 39.90
MOTA	3117	С	GLU		8	12.012	18.425		
ATOM	3118	ō	GLU		8			21.158	1.00 41.72
						12.189	17.359	21.733	1.00 41.52
ATOM	3119	CB	GLU		8	13.172	18.705	18.952	1.00 39.88
MOTA	3120	CG	GLU		8	14.037	19.626	18.090	1.00 41.02
MOTA	3121	CD	GLU	P	8	13.896	19.235	16.637	1.00 41.83
MOTA	3122	OE1	GLU	P	8	14.911	19.052	15.979	1.00 41.60
ATOM	3123	OE2	GLU	P	8	12.765	19.124	16.169	1.00 41.88
ATOM	3124	N	PHE		9	10.811	18.986		_
MOTA	3125	CA	PHE		9			21.162	1.00 45.62
ATOM						9.677	18.356	21.865	1.00 49.63
	3126	C	PHE		9	9.382	16.960	21.337	1.00 50.61
MOTA	3127	0	PHE	P	9	9.156	16.839	20.116	1.00 51.38
MOTA	3128	CB	PHE	P	9	8.451	19.245	21.670	1.00 50.65
ATOM	3129	CG	PHE	P	9	8.607	20.501	22.499	1.00 52.48
MOTA	3130	CD1	PHE	P	9	8.278	20.493	23.849	1.00 52.80
MOTA	3131		PHE		9	9.073	21.659	21.899	
ATOM	3132		PHE		9				1.00 53.12
ATOM	3133		PHE			8.420	21.651	24.600	1.00 53.74
					9	9.215	22.817	22.659	1.00 53.61
ATOM	3134	CZ	PHE		9	8.890	22.817	24.010	1.00 54.24
MOTA	3135	OXT	PHE		9	9.383	16.011	22.152	1.00 51.56
ATOM	3136	OH2	TIP	С	2	37.673	4.149	14.933	1.00 18.73
ATOM	3137	OH2	TIP	С	3	37.999	19.019	28.545	1.00 20.36
ATOM	3138	OH2	TIP	C	12	46.550	23.555	9.446	1.00 16.05
MOTA	3139		TIP		14	18.354	26.505		
ATOM	3140		TIP						
					15	33.073	10.884	15.835	1.00 14.30
ATOM	3141		TIP		16	15.032	34.698	31.070	1.00 11.96
ATOM	3142		TIP		17	7.170	35.908	33.277	1.00 16.70
MOTA	3143		TIP		19	16.624	32.704	28.166	1.00 15.10
MOTA	3144	OH2	TIP	С	20	35.078	42.552	29.609	1.00 19.72
ATOM	3145		TIP		21	40.457	30.360	27.755	1.00 16.31
MOTA	3146		TIP		22	52.263	20.430	9.725	· · · · ·
ATOM	3147		TIP		23	20.720			1.00 20.11
MOTA							20.412	14.822	1.00 12.68
	3148		TIP		24	33.413	15.317	~5.393	1.00 15.90
ATOM	3149		TIP		25	38.275	25.072	23.469	1.00 13.40
MOTA	3150		TIP		27	16.591	21.729	7.186	1.00 19.86
ATOM	3151	OH2	TIP	С	28	21.798	19.346	19.780	1.00 14.31
ATOM	3152		TIP		29	17.533	34.724	25.177	1.00 16.69
MOTA	3153		TIP		30	29.162	27.768	25.821	1.00 10.05
ATOM	3154	OH2			31	40.631			
ATOM	3155						28.021	16.946	1.00 14.53
		OH2			32	32.428	32.415	17.998	1.00 10.42
MOTA	3156	OH2			33	11.884	34.798	21.161	1.00 23.00
MOTA	3157	OH2			34	27.837	25.769	-5.173	1.00 33.18
MOTA	3158	OH2	TIP	C	35	12.372	31.279	28.339	1.00 16.96
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ATOM	3159	OH2	TIP C	36		39.263	28.648	25.755	1.00	9.84
ATOM	3160	OH2	TIP C	40		38.924	30.840	30.171	1 00	13.35
ATOM	3161.		TIP C	41		18.085	18.989	18.858		16.60
MOTA	3162	OH2	TIP C	42		7.300	35.692	30.168	1.00	19.22
MOTA	3163	OH2	TIP C	43		14.250	32.017	30.405	1.00	18.32
ATOM	3164	OH2	TIP C	44		37.440	22.761	1.333		23.96
ATOM	3165	OH2	TIP C	45		29.932	39.949	32.969		22.64
MOTA	3166	OH2	TIP C	46		29.433	17.902	20.935	1.00	16.15
ATOM	3167	OH2	TIP C	47		53.536	22.468	21.774	1.00	21.62
ATOM	3168	OH2		48		40.180	15.699	-0.272		12.15
ATOM	3169	OH2	TIP C	49		14.955	25.973	25.745		11.98
MOTA	3170	он2		50		38.595	6.527	3.885	1.00	23.66
MOTA	3171	OH2	TIP C	51		48.551	24.793	17.574	1.00	18.30
ATOM	3172	OH2	TIP C	52		20.747	27.407	17.869	1.00	8.25
ATOM	3173	OH2	TIP C	53		26.489	18.730	30.746		26.59
MOTA	3174	OH2	TIP C	54		38.723	11.162	19.249		11.49
MOTA	3175	OH2	TIP C	55		33.881	26.191	31.382	1.00	19.21
ATOM	3176	OH2	TIP C	56		13.322	31.213	40.027	1.00	15.61
MOTA	3177	OH2	TIP C	57		19.497	16.134	41.439	1.00	26.82
ATOM	3178	OH2	TIP C	58		38.469	37.062	5.695		23.10
						_				
ATOM	3179	OH2	TIP C	59		45.575	15.894	3.122		18.45
MOTA	3180	OH2	TIP C	60		39.615	25.333	-1.743	1.00	20.09
ATOM	3181	OH2	TIP C	61		32.158	37.928	32.431	1.00	12.17
ATOM	3182	OH2	TIP C	62		46.793	19.609	22.823	1.00	19.81
ATOM	3183		TIP C	63		24.847	37.031	-0.659		29.98
MOTA	3184		TIP C	64		45.957	18.715	3.836		18.88
MOTA	3185		TIP C	65		36.189	33.100	17.653		10.63
MOTA	3186	OH2	TIP C	66		31.177	25.020	24.150	1.00	28.40
MOTA	3187	OH2	TIP C	67		46.181	23.210	18.466	1.00	20.41
ATOM	3188		TIP C	68		21.756	10.923	7.943		22.80
MOTA	3189		TIP C	69		12.936	36.695	30.481		17.63
ATOM	3190	OH2	TIP C	70		33.713	44.843	8.382	1.00	30.49
MOTA	3191	OH2	TIP C	71		21.051	41.550	39.982	1.00	31.15
MOTA	3192	OH2	TIP C	72		26.815	38.732	3.198	1.00	22.61
ATOM	3193	OH2	TIP C	73		41.656	24.820	21.177	1.00	
			TIP C							31.08
MOTA	3194	OH2		74		25.521	30.139	47.617		
MOTA	3195	OH2	TIP C	75		20.497	46.537	15.336		29.67
MOTA	3196	OH2	TIP C	76		7.708	28.422	41.027	1.00	26.00
ATOM	3197	OH2	TIP C	77		25.650	18.585	27.821	1.00	17.30
MOTA	3198	он2	TIP C	78		35.124	16.582	21.374	1.00	15.44
ATOM	3199	OH2	TIP C	79		16.806	29.258	45.952		22.64
MOTA	3200		TIP C	80		29.365	7.305	14.767		28.00
MOTA	3201	OH2	TIP C	81		36.259	9.577	-0.018	1.00	36.72
MOTA	3202	OH2	TIP C	82		5.598	37.375	35 <i>.</i> 367	1.00	29.64
MOTA	3203	OH2	TIP C	83		14.256	22.267	9.863	1.00	20.30
ATOM	3204		TIP C	84		34.533	14.826	41.318		35.70
ATOM			TIP C							22.15
	3205			85		14.253	38.931	17.469		
MOTA	3206		TIP C	86		40.762	43.633	8.075		32.27
MOTA	3207	OH2	TIP C	87		20.139	38.471	47.202		19.79
ATOM	3208	OH2	TIP C	88		49.003	25.388	14.809	1.00	16.95
ATOM	3209		TIP C	89		48.376	21.580	21.346		26.51
ATOM	3210		TIP C	90		38.281	15.314	27.561		34.16
MOTA	3211		TIP C	91		8.631	39.984	34.095		41.37
MOTA	3212		TIP C	92		50.906	23.612	20.744		52.18
MOTA	3213	OH2	TIP C	93		53.785	20.060	24.538		24.16
ATOM	3214		TIP C	94		24.823	42.619	11.579		21.18
ATOM	3215		TIP C	95		25.075	45.083	6.146		38.65
				96		40.830				18.31
MOTA	3216		TIP C				25.584	18.443		
ATOM	3217		TIP C	97		43.416	22.239	18.182		19.16
MOTA	3218	OH2	TIP C	98		13.417	34.174	40.223		31.15
MOTA	3219	OH2	TIP C	99		33.278	34.940	35.258	1.00	19.39
MOTA	3220		TIP C	100	•	16.214	11.125	16.638		44.74
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ATOM	3221	OUR MED C	101				
		OH2 TIP C		53.364	20.723	14.579	1.00 34.15
ATOM	3222			49.883	22.898	7.975	1.00 17.76
ATOM	3223	OH2 TIP C	103	23.025	15.361	39.364	1.00 32.71
MOTA	3224	OH2 TIP C	104	9.989	41.920	29.368	
MOTA	3225	OH2 TIP C					1.00 18.54
MOTA				40.434	26.276	24.857	1.00 17.36
	3226	OH2 TIP C		20.997	29.964	6.095	1.00 20.90
MOTA	3227	OH2 TIP C		27.762	47.336	16.035	1.00 24.48
ATOM	3228	OH2 TIP C	108	49.284	22.771	5.126	1.00 18.73
ATOM	3229	OH2 TIP C		48.838	23.239	29.592	
ATOM	3230	OH2 TIP C					1.00 33.97
				28.582	23.099	35.349	1.00 20.25
ATOM	3231	OH2 TIP C		32.528	35.162	39.110	1.00 29.39
MOTA	3232	OH2 TIP C	112	41.404	21.066	27.696	1.00 29.24
MOTA	3233	OH2 TIP C	113	41.566	30.795	24.916	1.00 29.04
ATOM	3234	OH2 TIP C		38.888	34.349		
ATOM	3235	OH2 TIP C				4.634	1.00 19.24
ATOM				21.524	13.318	6.181	1.00 21.83
	3236	OH2 TIP C		20.262	44.365	41.166	1.00 51.68
MOTA	3237	OH2 TIP C		40.866	37.586	7.262	1.00 26.48
MOTA	3238	OH2 TIP C	118	24.269	19.013	20.381	1.00 20.56
ATOM	3239	OH2 TIP C	119	14.796	40.366	21.026	1.00 26.21
ATOM	3240	OH2 TIP C		40.271			
ATOM	3241	OH2 TIP C			21.968	24.452	1.00 22.99
				27.256	8.206	3.568	1.00 32.16
MOTA	3242	OH2 TIP C		38.453	23.426	21.155	1.00 20.65
ATOM	3243	OH2 TIP C	123	39.489	30.192	18.787	1.00 19.64
ATOM	3244	OH2 TIP C	124	49.479	24.877	3.120	1.00 15.38
MOTA	3245	OH2 TIP C		23.534	17.922		
ATOM	3246	OH2 TIP C				36.838	1.00 21.55
				24.481	13.568	37.531	1.00 33.00
ATOM	3247	OH2 TIP C		27.515	37.075	45.132	1.00 32.65
ATOM	3248	OH2 TIP C		20.903	11.530	10.774	1.00 25.13
ATOM	3249	OH2 TIP C	129	16.996	37.117	6.834	1.00 26.72
ATOM	3250	OH2 TIP C		42.280	39.848	5.806	
MOTA	3251	OH2 TIP C					1.00 39.08
				15.426	37.238	14.643	1.00 27.36
ATOM	3252	OH2 TIP C		47.740	29.973	16.321	1.00 27.58
MOTA	3253	OH2 TIP C		52.162	19.864	18.278	1.00 19.10
ATOM	3254	OH2 TIP C	134	47.805	11.416	4.529	1.00 30.40
ATOM	3255	OH2 TIP C	135	20.920	22.905	41.964	1.00 23.80
ATOM	3256	OH2 TIP C		27.784	19.013	-1.506	
ATOM	3257	OH2 TIP C	137				1.00 28.71
				25.506	36.437	2.115	1.00 19.53
ATOM	3258		138	6.347	36.058	44.801	1.00 30.54
ATOM	3259	OH2 TIP C		18.428	23.862	8.397	1.00 19.65
ATOM	3260	OH2 TIP C	140	56.631	14.945	24.048	1.00 29.26
MOTA	3261	OH2 TIP C	141	36.045	33.381	-3.424	1.00 39.63
ATOM	3262	OH2 TIP C		20.242	14.180		
ATOM	3263	OH2 TIP C				11.802	1.00 31.49
ATOM				8.614		31.526	1.00 30.94
	3264	OH2 TIP C		8.697	38.736	31.440	1.00 44.64
MOTA	3265	OH2 TIP C		21.002	20.115	40.621	1.00 23.34
ATOM	3266	OH2 TIP C	146	36.343	37.533	7.628	1.00 25.43
ATOM	3267	OH2 TIP C	147	13.944	44.970	51.125	1.00 40.01
ATOM	3268	OH2 TIP C		12.509	22.964		
MOTA	3269	OH2 TIP C				23.735	1.00 33.44
				32.555	6.398	6.686	1.00 30.50
ATOM	3270	OH2 TIP C		11.123	30.018	41.695	1.00 29.12
MOTA	3271	OH2 TIP C		20.406	19.454	17.419	1.00 26.72
ATOM	3272	OH2 TIP C	152	37.729	21.375	25.750	1.00 27.16
ATOM	3273	OH2 TIP C		36.922	28.170	33.507	1.00 42.28
ATOM	3274	OH2 TIP C		13.904			
ATOM	3275				29.766	32.277	1.00 19.72
		OH2 TIP C		54.556	19.732	11.775	1.00 37.67
MOTA	3276	OH2 TIP C		14.999	28.327	48.310	1.00 40.64
MOTA	3277	OH2 TIP C	157	19.001	46.759	12.106	1.00 40.48
MOTA	3278	OH2 TIP C	158	22.361	9.339	13.691	1.00 44.57
ATOM	3279	OH2 TIP C		26.097	16.601		
ATOM	3280	OH2 TIP C		51.862		36.996	1.00 27.61
ATOM	3281				24.669	14.501	1.00 39.22
		OH2 TIP C		42.713	33.316	38.299	1.00 37.21
ATOM	3282	OH2 TIP C	T07	32.074	43.316	6.583	1.00 32.14

MOTA	3283	OH2	TIP (163	44.434	22.056	2.693	1.00 44.76
ATOM	3284	OH2	TIP (: 164	24.074	33.090	45.770	1.00 26.95
ATOM	3285	он2	TIP (165		35.656	48.500	1.00 33.30
ATOM	3286		TIP (27.253	51.538	1.00 48.93
ATOM	3287	OH2	TIP (14.390	20.410	
,								1.00 32.12
MOTA	3288		TIP (34.543	25.107	1.00 34.11
ATOM	3289		TIP (33.697	5.939	1.00 29.72
ATOM	3290	OH2	TIP (: 170	26.378	23.008	46.449	1.00 37.54
ATOM	3291	OH2	TIP (: 171	10.530	41.770	49.010	1.00 34.66
MOTA	3292	OH2	TIP (: 172	41.154	5.586	4.533	1.00 25.18
ATOM	3293	он2	TIP (: 173		11.487	4.521	1.00 46.32
ATOM	3294		TIP (39.527	37.113	1.00 36.37
ATOM	3295		TIP (23.235	37.583	1.00 39.37
ATOM	3296			-				
			TIP (21.891	40.191	1.00 36.81
ATOM	3297		TIP (26.159	40.588	1.00 38.22
MOTA	3298		TIP (29.183	54.400	1.00 39.76
ATOM	3299		TIP (47.986	22.417	1.00 32.19
ATOM	3300	OH2	TIP (: 180	37.394	44.558	11.594	1.00 39.03
MOTA	3301	OH2	TIP (: 181	53.552	27.209	11.822	1.00 47.97
MOTA	3302	OH2	TIP (: 182	10.503	32.709	12.025	1.00 38.41
MOTA	3303	OH2	TIP (: 183	17.985	14.916	28.259	1.00 36.86
MOTA	3304	OH2				45.446	12.174	1.00 49.92
ATOM	3305		TIP (15.741	36.532	1.00 40.29
ATOM	3306		TIP (22.471	17.335	1.00 40.23
MOTA	3307		TIP (
						28.369	50.282	1.00 42.57
ATOM	3308		TIP (14.816	0.037	1.00 36.60
MOTA	3309		TIP (26.536	23.386	1.00 44.75
MOTA	3310		TIP (17.794	24.745	1.00 42.51
MOTA	3311	OH2	TIP (: 191		32.293	36.650	1.00 38.36
MOTA	3312	OH2	TIP (: 192	30.315	9.929	15.860	1.00 39.58
MOTA	3313	OH2	TIP (: 193	29.613	40.378	2.225	1.00 41.26
ATOM	3314	OH2	TIP (: 194	14.241	43.934	16.316	1.00 43.60
MOTA	3315	OH2	TIP (: 195	48.673	31.215	7.801	1.00 32.67
MOTA	3316		TIP (21.963	18.969	1.00 41.87
ATOM	3317		TIP (39.077	3.714	1.00 35.77
ATOM	3318	OH2				11.993	21.654	1.00 38.05
ATOM	3319		TIP			31.378	4.946	1.00 48.02
ATOM	3320	OH2				46.520	15.659	1.00 45.30
ATOM	3321		TIP (40.320	40.154	1.00 40.62
ATOM	3322							
ATOM	3323		TIP (18.652	7.189	1.00 43.28
		OH2				17.526	41.765	1.00 61.21
MOTA	3324		TIP (36.523	-0.637	1.00 43.56
MOTA	3325		TIP (29.974		1.00 47.33
MOTA	3326		TIP (37.731	18.949	1.00 44.12
ATOM	3327		TIP (26.744	22.711	1.00 40.03
ATOM	3328	OH2	TIP (208	9.555	36.540	23.357	1.00 46.94
MOTA	3329	OH2	TIP (209	23.046	47.732	4.343	1.00 48.13
MOTA	3330	ОН2	TIP (210		44.592	5.460	1.00 64.51
MOTA	3331		TIP (41.071	6.267	1.00 48.35
ATOM	3332		TIP (46.493	17.139	1.00 39.09
ATOM	3333		TIP (17.658	1.00 43.06
ATOM	3334		TIP (35.093	42.826	1.00 38.97
ATOM	3335		TIP (14.910	43.677	1.00 44.01
ATOM	3336		TIP (23.673	44.607	1.00 45.50
MOTA	3337		TIP (35.555	7.510	1.00 29.79
ATOM	3338		TIP (25.648	42.564	1.00 56.65
MOTA	3339		TIP (8.547	20.446	1.00 47.85
MOTA	3340	OH2	TIP (220	-0.925	31.171	41.173	1.00 36.99
ATOM	3341	OH2	TIP (221	41.791	22.878	0.132	1.00 56.14
MOTA	3342		TIP (25.685	41.540	1.00 47.43
ATOM	3343		TIP (4.785	13.582	1.00 47.96
MOTA	3344		TIP (4.520	15.174	1.00 48.76
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MOTA	3345	OH2	TIP (225	10.029	32.425	18.562	1.00 36.30
MOTA	3346	OH2	TIP (226	22.346	37.737	48.941	1.00 34.15
MOTA	3347.	OH2	TIP (227	16.274	17.012	19.693	1.00 27.63
ATOM	3348	OH2	TIP (228	35.332	13.692	20.375	1.00 37.59
MOTA	3349	OH2	TIP (229	41.228	36.673	22.908	1.00 51.58
ATOM	3350	OH2	TIP (230	17.416	42.030	50.226	1.00 47.63
ATOM	3351	OH2	TIP (231	18.428	39.213	52.835	1.00 40.43
ATOM	3352	OH2			42.243	43.386	25.548	1.00 48.60
ATOM	3353	OH2			14.081	18.701	0.364	
ATOM	3354	OH2			41.421	41.332		1.00 32.87
ATOM	3355	OH2	TIP (42.772	36.396	28.531 11.892	1.00 54.67
ATOM	3356	OH2			13.068	13.733		1.00 41.24
ATOM.	3357 ·						28.653	1.00 42.66
ATOM	3358	OH2	TIP (10.850	26.738	7.811	1.00 40.46
ATOM	3359	OH2	TIP (16.253	20.926	45.776	1.00 44.60
ATOM	3360	OH2			32.681	31.139	43.220	1.00 42.20
ATOM	3361	OH2	TIP (56.267	22.254	9.280	1.00 52.44
ATOM	3362				12.553	25.304	9.942	1.00 38.77
ATOM		OH2			50.727	9.516	16.775	1.00 33.38
ATOM	3363 3364	OH2	TIP C		31.871	41.347	0.512	1.00 47.78
ATOM		OH2	TIP (10.008	45.092	37.807	1.00 39.52
	3365	OH2	TIP C		14.551	39.030	6.708	1.00 44.26
ATOM	3366	OH2	TIP C		26.955	18.903	-5.135	1.00 42.54
ATOM	3367	OH2	TIP C		39.916	22.478	18.854	1.00 33.22
MOTA	3368	OH2	TIP (40.431	40.824	22.426	1.00 35.58
ATOM	3369		TIP C		52.081	23.408	10.759	1.00 42.53
ATOM	3370		TIP C		12.078	16.710	24.149	1.00 32.37
ATOM	3371		TIP C		54.111	15.908	8.256	1.00 44.58
MOTA	3372	OH2	TIP C		33.950	12.827	-1.753	1.00 27.02
MOTA	3373	OH2	TIP C		-0.775	26.703	40.353	1.00 43.64
ATOM	3374	OH2	TIP C		1.937	33.711	40.561	1.00 42.67
ATOM	3375		TIP C		8.008	24.066	18.824	1.00 51.45
ATOM	3376	OH2	TIP C	256	11.765	27.465	3.635	1.00 47.34
MOTA	3377		TIP C		27.863	43.878	9.233	1.00 32.44
MOTA	3378	OH2	TIP C		18.655	30.114	4.303	1.00 33.13
MOTA	3379	OH2	TIP C		21.592	19.085	-3.960	1.00 39.86
ATOM	3380	OH2			41.876	24.067	25.906	1.00 26.34
MOTA	3381	OH2	TIP C	261	46.651	10.240	2.171	1.00 44.38
ATOM	3382		TIP C		32.536	15.827	32.477	1.00 43.28
MOTA	3383	OH2	TIP C	263	12.479	39.205	50.359	1.00 47.33
MOTA	3384	OH2	TIP C		0.850	27.980	38.316	1.00 43.45
MOTA	3385	OH2			49.605	7.356	18.061	1.00 66.01
MOTA	3386		TIP C		30.177	40.365	-3.235	1.00 44.45
ATOM	3387	OH2	TIP C	267	39.818	12.364	0.512	1.00 48.84
ATOM	3388		TIP C		38.149	44.716	27.884	1.00 51.18
MOTA	3389		TIP C		37.156	37.062	30.528	1.00 35.17
MOTA	3390		TIP C		51.808	7.097	12.435	1.00 51.69
MOTA	3391		TIP C		54.351	12.626	12.471	1.00 47.45
MOTA	3392		TIP C		50.835	31.155	13.092	1.00 55.05
MOTA	3393		TIP C		12.159	35.313°	52.133	1.00 52.38
MOTA	3394		TIP C		21.002	44.489	13.037	1.00 39.70
ATOM	3395	OH2	TIP C	275	37.936	23.627	34.221	1.00 48.56
MOTA	3396		TIP C			30.935	31.365	1.00 43.24
MOTA	3397	OH2	TIP C	277	38.831	48.015	15.554	1.00 49.83
	3398	OH2	TIP C	278	5.630	28.150	44.576	1.00 48.10
MOTA	3399		TIP C		8.600	24.000	45.727	1.00 49.27
MOTA	3400		TIP C		54.276	20.854	7.807	1.00 36.02
ATOM	3401		TIP C		3.544	34.696	46.365	1.00 43.63
ATOM	3402		TIP C		24.214	46.264	46.163	1.00 48.04
ATOM	3403		TIP C		7.099	32.072	19.549	1.00 54.97
ATOM	3404		TIP C		36.469	22.374	41.355	1.00 52.17
MOTA	3405		TIP C		34.660	13.757	23.756	1.00 45.46
MOTA	3406		TIP C		28.516	42.981	5.402	1.00 53.58
								22.00

MOTA	3407	OH2	TIP C	287	35.579	4.929	12.012	1.00 52.07
ATOM	3408	OH2	TIP C	288	22.974	49.682	24.299	1.00 53.67
MOTA	3409	OH2	TIP C	289	3.725	31.464	46.354	1.00 46.43
ATOM	3410		TIP C		27.340	39.594	-2.191	1.00 56.89
MOTA	3411		TIP C		33.413	34.856	32.335	1.00 31.78
ATOM	3412	OH2	TIP C	292	43.340	7.715	8.063	1.00 43.53
ATOM	3413	OH2	TIP C	293	28.243	21.392	-4.937	1.00 38.33
ATOM	3414	OH2	TIP C	294	49.389	26.590	35.796	1.00 45.66
ATOM	3415		TIP C		28.948	15.824	33.796	1.00 52.48
ATOM	3416		TIP C		27.347	13.383	37.207	1.00 48.27
ATOM	3417	OH2	TIP C	297	38.485	26.090	36.901	1.00 48.92
ATOM	3418	OH2	TIP C	298	12.120	20.265	11.506	1.00 50.10
ATOM	3419	OH2	TIP C	299	36.480	36.306	38.613	1.00 50.38
ATOM	3420		TIP C		31.471	16.463	35.507	1.00 38.37
MOTA	3421		TIP C		42.889	5.274	2.358	1.00 33.49
MOTA	3422		TIP C		23.548	44.173	32.246	1.00 39.09
MOTA	3423	OH2	TIP C	303	13.465	43.978	13.054	1.00 52.67
ATOM	3424	OH2	TIP C	304	25.133	43.053	4.111	1.00 52.03
ATOM	3425		TIP C	305	33.587	24.652	39.392	1.00 49.48
ATOM	3426		TIP C		39.063	28.353	1.979	1.00 47.89
MOTA	3427			307	49.357	35.834	12.150	1.00 49.22
ATOM	3428	OH2	TIP C	308	27.159	46.386	33.347	1.00 49.50
ATOM	3429	OH2	TIP C	309	9.510	21.769	39.704	1.00 47.95
ATOM	3430	OH2	TIP C	310	34.885	32.959	39.205	1.00 51.26
ATOM	3431		TIP C		30.980	6.002	9.747	1.00 56.02
					43.802			
MOTA	3432		TIP C			34.511	14.853	1.00 41.89
MOTA	3433		TIP C		36.834	4.382	5.254	1.00 39.04
MOTA	3434	OH2	TIP C	314	12.453	30.429	47,461	1.00 47.60
MOTA	3435	OH2	TIP C	315	39.685	40.144	30.944	1.00 54.68
MOTA	3436	OH2	TIP C	316	45.982	20.840	31.078	1.00 47.99
ATOM	3437		TIP C		32.815	36.023	42.050	1.00 45.07
MOTA	3438	_	TIP C		17.877	37.802	-3.699	1.00 56.30
ATOM	3439	OH2	TIP C	319	53.681	9.633	16.525	1.00 55.34
ATOM	3440	OH2	TIP C	320	21.577	43.070	52.229	1.00 49.54
ATOM	3441	OH2	TIP C	321	6.139	45.122	36.565	1.00 44.40
ATOM	3442	OH2	TIP C	322	34.695	13.561	26.782	1.00 45.99
ATOM	3443		TIP C		17.990	33.946	-9.976	1.00 56.88
			TIP C		25.587			1.00 52.75
ATOM	3444					50.416	28.268	
ATOM	3445		TIP C		27.744	42.608	42.266	1.00 44.66
MOTA	3446		TIP C	326	48.357	32.815	33.851	1.00 57.98
MOTA	3447	OH2	TIP C	327	61.047	18.004	17.692	1.00 51.30
ATOM	3448	OH2	TIP C	328	17.327	11.069	11.972	1.00 48.28
ATOM	3449		TIP C		59.624	17.562	20.598	1.00 44.37
ATOM	3450		TIP C		40.644	39.227	19.932	1.00 37.57
MOTA	3451		TIP C		12.920	31.214	52.942	1.00 51.07
ATOM	3452		TIP C		37.639	0.847	19.561	1.00 49.44
ATOM	3453		TIP C		34.243	38.790	-3.251	1.00 54.21
ATOM	3454	OH2	TIP C	334	24.216	47.874	6.983	1.00 50.90
MOTA	3455		TIP C		15.324	34.797	6.670	1.00 45.25
ATOM	3456		TIP C		18.474	15.525	21.402	1.00 34.12
								1.00 49.89
ATOM	3457		TIP C		40.048	8.873	26.818	
ATOM	3458		TIP C		32.472	13.331	20.523	1.00 29.86
MOTA	3459	он2	TIP C	339	57.778	14.167	30.422	1.00 49.76
ATOM	3460	OH2	TIP C	340	46.651	35.476	13.375	1.00 56.48
ATOM	3461		TIP C		15.427	13.237	3.552	1.00 57.25
ATOM	3462		TIP C		40.349	38.972	3.722	1.00 65.27
								1.00 59.60
ATOM	3463		TIP C		8.685	28.945	15.205	
ATOM	3464		TIP C		11.958	41.585	22.587	1.00 37.18
MOTA	3465		TIP C		9.054	20.498	28.914	1.00 42.95
ATOM	3466	OH2	TIP C	346	20.086	20.088	46.913	1.00 42.03
ATOM	3467	он2	TIP C	347	40.370	35.093	2.009	1.00 49.35
ATOM	3468		TIP C		41.948	4.327	12.147	1.00 50.59
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INTERNATIONAL SEARCH REPORT

International application No.

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A. CLASSIFICATION OF SUBJECT MATTER IPC(7) : G01N 33/483								
US ČĹ : 702/19								
	International Patent Classification (IPC) or to both I	national classification and IPC						
B. FIEL	DS SEARCHED		•					
Minimum documentation searched (classification system followed by classification symbols) U.S.: 702/17, 435, 424.								
Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched								
Electronic data base consulted during the international search (name of data base and, where practicable, search terms used) Please See Continuation Sheet								
	UMENTS CONSIDERED TO BE RELEVANT							
Category *	Citation of document, with indication, where a		Relevant to claim No.					
Y	ROSSIOHN et al. Crystal structure of the N-terminal, growth factor-like domain of Alzheimer amyloid precursor protein. Nature Structural Biology. April 1999, Vol 6. No. 4, pages 327-331, see entire document and especially page 330 in Methods.							
Y	ZHANG Z. et al. Sequence-specific recognition of the interanalization motif of the Alzheimer's amyloid precursor protein by the X11 PTB domain. The EMBO Journal. 1997, Vol 16. No. 20, pages 6141-6150, see entire document and especially page 6147.							
Y,P	MARCINKEVICIENE J. at al. Mechanism of Inhibition of beta-Site Amyloid Precursor Protein-cleaving Enzyme (BACE) by a Statine-based Peptide. The Journal of Biological Chemistry. 29 June 2001, Vol 276, No. 26, pages 23790-23794, see entire document.							
Y	HYNES et al. X-ray Crystal Structure of the Protea Amyloid beta-Protein Precursor. Biochemistry. 1990 especially page 10019.	1-2						
Further	documents are listed in the continuation of Box C.	See patent family annex.						
	pecial categories of cited documents:		mational filing date or priority					
"A" document defining the general state of the art which is not considered to be date and not in conflict with the application but cited to understand to principle or theory underlying the invention								
of particular relevance "X" document of particular relevance; the claimed invention "E" earlier application or patent published on or after the international filing date considered novel or cannot be considered to involve an when the document is taken alone								
establish specified)		"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination						
"O" document	referring to an oral disclosure, use, exhibition or other means	being obvious to a person skilled in the	e art					
"P" document published prior to the international filing date but later than the "&" document member of the same patent family priority date claimed								
Date of the actual completion of the international search Date of mailing of the international search report 13 F EB 2002								
18 December 2001 (18.12.2001)								
Name and mailing address of the ISA/US Commissioner of Patents and Trademarks								
Box PCT Washington, D.C. 20231 NI Koca M. GALIZZEN PhD								
Facsimile No	o. (703)305-3230	Telephone No. (703)-308-0196	101/4 . Um.					
Form PCT/ISA/210 (second sheet) (July 1998)								

INTERNATIONAL SEARCH REPORT

International application No.

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tegory *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.	
Y	BAILEY et al. X-ray-crystallographic studies of complexes of pepstatin A and a statine-containing human renin inhibitor with endothiapepsin. Biochem. J.1993, Vol 289, pages 363-371, especially pages 365-366.	1-2	
Y	SCHEIDIG et al. Crystal structures of bovin chymotrypsin and trypsin complexed to the inhibitor domain of Alzheimer's amyloid beta-protein precursor (APPI) and basic pancreatic trypsin inhibitor (BPTI): Engineering of inhibitors with altered specificities. The Protein Society. September 1997, Vol 6, pages 1806-1824, see entire document and especially page 1820.	1-2	
A	KOHNO et al. Thre-Dimentional Structure of the Amyloid beta Peptide (25-35) in Membrane-Mimicking Environment. Biochemistry. 1996, Vol 35, pages 16094-16104, see entire document.	1-2	
A	VASSAR et al. Beta-Secretase Cleavage of Azheimer's Amyloid Precursor Protein by the Transmembrane Aspartic Protease BACE. Science. 22 October 1999, Vol 286, pages 735-741, see entire document.	1-2	
A	HONG, L. et al. Structure of the Protease Domain of Memapsin 2(beta-Secretase) Complexed with Inhibitor. Science. 24 May 2000, Vol 290, No. 5489, pages 150-159, see entire document	1-2	
A	SAUDER, M. et al. Modeling of substrate specifity of the Alzheimer's desease amyloid precursor protein beta-secretase. J. Mol. Biol. 2000, Vol 300, No. 2, pages 241-248, see entire document.	1-2	
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INTERNATIONAL SEARCH REPORT

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Box I Observations where certain claims were found unsearchable (Continuation of Item 1 of first sheet)						
This international report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:						
1. Claim Nos.: because they relate to subject matter not required to be searched by this Authority, namely:						
Claim Nos.: because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:						
3. Claim Nos.: because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).						
Box II Observations where unity of invention is lacking (Continuation of Item 2 of first sheet)						
This International Searching Authority found multiple inventions in this international application, as follows: Please See Continuation Sheet						
1. As all required additional search fees were timely paid by the applicant, this international search report covers all searchable claims.						
2. As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.						
3. As only some of the required additional search fees were timely paid by the applicant, this international search report covers only those claims for which fees were paid, specifically claims Nos.: 1 and 2						
4. No required additional search fees were timely paid by the applicant. Consequently, this international search report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:						
Remark on Protest The additional search fees were accompanied by the applicant's protest. No protest accompanied the payment of additional search fees.						

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BOX II. OBSERVATIONS WHERE UNITY OF INVENTION IS LACKING

The inventions listed as Groups I-II do not relate to a single general inventive concept under PCT Rule 13.1 because, under PCT Rule 13.2, they lack the same or corresponding special technical features for the following reasons:

The inventions listed as Groups I-II do not relate to a single general inventive concept under PCT Rule 13.1 because, under PCT Rule 13.2, they lack the same or corresponding special technical features for the following reasons: Invention I and II are directed to different chemical and physical types regarding the critical limitations therein. For Group I, the critical feature is a crystallization of complex whereas for Group II the critical feature is the obtaining or synthesizing the agent. This application contains the following inventions or groups of inventions which are not so linked as to form a single general inventive concept under PCT Rule 13.1. In order for all inventions to be searched, the appropriate additional examination fees must be paid.

Group I, claims 1-2, drawn to crystallized complex.

Group II, claims 24 and 27 drawn to method further comprising one of the steps: obtaining and synthesizing the agen. Claims 3-23, 25,26,28-30 are directed solely to information and are therefore excluded from search.

The International Searching Authority considers that the international application does not comply with the requirements of unity of invention (Rules 13.1, 13.2 and 13.3) for reasons indicated below:

The inventions listed as Groups I-II do not relate to a single general inventive concept under PCT Rule 13.1 because, under PCT Rule 13.2, they lack the same or corresponding special technical features for the following reasons:

The inventions listed as Groups I-II do not relate to a single general inventive concept under PCT Rule 13.1 because, under PCT Rule 13.2, they lack the same or corresponding special technical features for the following reasons: Invention I and II are directed to different chemical and physical types regarding the critical limitations therein. For Group I, the critical feature is a crystallization of complex whereas for Group II the critical feature is the obtaining or synthesizing the agent.

Continuation of B. FIELDS SEARCHED Item 3:

WEST, STN, Non-patent-literature covering search terms: Cleaving Enzyme(BACE), crystallization, beta-Amyloid Precursor protein, 3-d structure of APP, Statine-based peptides.